Supplementary Materials

Kinetics and General Reaction Rules for Hydrogen Atom Abstraction Reactions from C4−C7 Oxygenated Fuels by Hydroxyl Radical

Ying Huo [a], *Yachao Chang* [a,*], *Lili Ye* [b], *Ming Jia* [a,*]

[a] Key Laboratory of Ocean Energy Utilization and Energy Conservation of Ministry of Education, Dalian University of Technology, Dalian, Liaoning 116024, P.R. China

[b] School of Chemical Engineering, Dalian University of Technology, Dalian, Liaoning 116024, P.R. China

S1 Relative energies of the H-abstraction reactions

Table S1. Relative energies of the H-abstraction reactions of $C_nH_{2n+1}COOCH_3$ (n = 2–3), $C_nH_{2n+1}C(O)CH_3$ (n = 2–3), $C_nH_{2n+1}OCH_3$ (n = 3–4), and $C_nH_{2n+1}CHO$ (n = 3–4) with HȮ using the M062x/6-311++G (d, p) and CCSD(T) methods

Molecular system	M06-2x (kcal/mol)	CCSD(T) (kcal/mol)	Difference (kcal/mol)	Molecular system	M06-2x (kcal/mol)	CCSD(T) (kcal/mol)	Difference (kcal/mol)
$C_2H_5COOCH_3$+OH	0.00	0.00	0.00	EP1’	-22.54	-21.91	0.63
ER1	-4.48	-3.28	1.20	EP1	-22.54	-21.91	0.63
ER2	-6.50	-4.78	1.72	EP2	-28.81	-28.21	0.60
ER3	-4.58	-3.19	1.39	EP3	-20.97	-20.67	0.30
ER4	-6.58	-4.90	1.68	EP3’	-17.48	-17.43	0.05
TS1’	3.25	4.10	0.85	P1’	-18.19	-19.82	1.63
TS1	-0.43	0.56	0.99	P1	-18.20	-19.83	1.63
TS2	0.38	1.07	0.69	P2	-24.45	-25.21	0.76
TS3	-0.60	0.45	1.05	P3	-16.13	-17.65	1.52
TS3’	2.65	2.88	0.23	P3’	-15.03	-16.27	1.24
$C_3H_7COOCH_3$+OH	0.00	0.00	0.00	EP1	-22.56	-21.95	0.61
ER1	-4.49	-3.32	1.17	EP2	-28.29	-27.62	0.97
ER2	-6.51	-4.81	1.70	EP3	-24.63	-23.47	1.16
ER3	-4.60	-3.25	1.35	EP4	-19.87	-19.67	0.20
ER4	-6.72	-5.04	1.68	EP4’	-18.27	-18.54	0.27
TS1’	3.21	4.06	0.85	P1’	-18.19	-19.83	1.64
TS1	-0.42	0.56	0.98	P1	-18.19	-19.83	1.64
TS2	0.15	0.73	0.58	P2	-23.94	-24.59	0.65
TS3	-2.40	-1.57	0.83	P3	-19.38	-20.46	1.08
TS4	1.54	2.01	0.47	P4	-16.57	-18.05	1.48
TS4’	2.34	2.65	0.31	P4’	-16.27	-17.68	1.41
EP1’	-22.56	-21.95	0.61				
$C_3H_7OCH_3$+OH	0.00	0.00	0.00	EP2	-27.24	-26.30	0.94
ER1	-6.74	-5.31	1.43	EP3	-24.45	-23.35	1.10
TS1’	1.52	2.48	0.96	EP4	-19.37	-19.41	0.04
TS1	0.44	0.75	0.31	EP4’	-18.39	-18.69	0.30
TS2	-0.90	-0.54	0.36	P1’	-21.19	-23.11	1.92
TS3	-1.80	-0.76	1.04	P1	-21.18	-23.10	1.92
TS4	1.74	2.20	0.46	P2	-22.58	-24.05	1.47
TS4’	2.44	2.79	0.35	P3	-18.50	-19.78	1.28
EP1’	-25.79	-25.79	0.00	P4	-16.61	-18.06	1.45
EP1	-25.80	-25.79	0.01	P4’	-16.51	-17.91	1.40
$C_4H_9OCH_3$+OH	0.00	0.00	0.00	EP3	-25.37	-23.88	1.49
ER1	-6.76	-5.38	1.38	EP4	-22.81	-22.47	0.34
TS1’	1.54	2.48	0.94	EP5	-19.41	-19.21	0.20
TS1	0.41	0.72	0.31	EP5’	-18.72	-19.01	0.29
TS2	-0.87	-0.54	0.33	P1’	-21.17	-23.09	1.92

Table S1 Continue

Molecular system	M06-2x (kcal/mol)	CCSD(T) (kcal/mol)	Difference (kcal/mol)	Molecular system	M06-2x (kcal/mol)	CCSD(T) (kcal/mol)	Difference (kcal/mol)
TS3	-2.01	-1.08	0.93	P1	-21.17	-23.09	1.92
TS4	0.30	0.62	0.32	P2	-22.64	-24.09	1.45
TS5	1.64	2.15	0.51	P3	-18.21	-19.44	1.23
TS5’	2.18	2.38	0.20	P4	-19.67	-20.72	1.05
EP1’	-25.78	-26.29	0.51	P5	-16.54	-18.04	1.50
EP1	-25.83	-25.85	0.02	P5’	-16.27	-17.70	1.43
EP2	-26.59	-26.66	0.07				
$C_2H_5C(O)CH_3$+OH	0.00	0.00	0.00	EP2	-32.85	-31.48	1.37
ER1	-6.36	-	-	EP3	-21.43	-19.92	1.51
ER2	-6.63	-4.69	1.94	EP3’	-18.07	-17.72	0.35
TS1	1.09	2.19	1.10	P1	-21.17	-21.71	0.54
TS2	0.66	1.15	0.49	P2	-26.83	-26.87	0.04
TS3	-0.73	0.65	1.38	P3	-16.19	-17.43	1.24
TS3’	2.30	2.86	0.56	P3’	-15.33	-16.31	0.98
EP1	-27.59	-26.76	0.83				
$C_3H_7C(O)CH_3$+OH	0.00	0.00	0.00	EP2	-32.32	-31.22	1.10
ER1	-6.39	-	-	EP3	-24.81	-23.55	1.26
ER2	-6.81	-5.15	1.66	EP4	-20.29	-20.13	0.16
TS1	1.01	1.82	0.81	EP4’	-18.48	-18.71	0.23
TS2	0.27	0.53	0.26	P1	-21.22	-22.02	0.80
TS3	-2.53	-1.64	0.89	P2	-26.28	-26.49	0.21
TS4	1.30	1.81	0.51	P3	-19.42	-20.51	1.09
TS4’	2.21	2.54	0.33	P4	-16.64	-18.11	1.47
EP1	-27.72	-27.17	0.55	P4’	-16.47	-17.88	1.41
C_3H_7CHO+OH	0.00	0.00	0.00	EP2	-33.79	-32.20	1.59
ER1	-3.11	-2.11	1.00	EP3	-24.66	-23.39	1.27
ER2	-6.22	-4.59	1.63	EP4	-20.14	-19.91	0.23
TS1	-1.87	-1.20	0.67	EP4’	-18.23	-18.48	0.25
TS2	1.15	1.35	0.20	P1	-28.08	-30.12	2.02
TS3	-1.97	-1.11	0.86	P2	-27.43	-27.49	0.06
TS4	1.44	1.97	0.53	P3	-19.59	-20.70	1.11
TS4’	2.39	2.72	0.33	P4	-16.57	-18.04	1.47
EP1	-31.67	-32.21	0.54	P4’	-16.37	-17.77	1.40
C_4H_9CHO+OH	0.00	0.00	0.00	EP3	-25.52	-24.30	1.22
ER1	-5.03	-4.44	0.59	EP4	-23.51	-22.96	0.55
ER2	-6.35	-4.64	1.71	EP5	-19.79	-19.41	0.38
TS1	-1.89	-1.22	0.67	EP5’	-18.67	-18.53	0.14
TS2	1.05	1.26	0.21	P1	-28.08	-30.13	2.05
TS3	-2.31	-1.49	0.82	P2	-27.65	-27.70	0.05
TS4	-0.10	0.31	0.41	P3	-19.22	-20.32	1.10
TS5	1.55	2.08	0.53	P4	-19.64	-20.72	1.08

Table S1 Continue

Molecular system	M06-2x (kcal/mol)	CCSD(T) (kcal/mol)	Difference (kcal/mol)	Molecular system	M06-2x (kcal/mol)	CCSD(T) (kcal/mol)	Difference (kcal/mol)
TS5’	2.15	2.35	0.20	P5	-16.50	-18.00	1.50
EP1	-31.70	-32.26	0.56	P5’	-16.25	-17.68	1.43
EP2	-34.92	-32.88	2.04				

Table S2. Mean absolute errors (MAE) and maximum deviations for energy barriers and reaction energies compared to CCSD(T)/CBS benchmark

Fuel class	Energy type	MAE (kcal/mol)	Max deviation (kcal/mol)
Esters (C4-C5)	Energy barrier	0.71	1.05
	Reaction energy	1.33	1.64
Ethers (C4-C5)	Energy barrier	0.54	1.04
	Reaction energy	1.53	1.92
Ketones (C4-C5)	Energy barrier	0.70	1.38
	Reaction energy	0.86	1.47
Aldehydes (C4-C5)	Energy barrier	0.49	0.86
	Reaction energy	1.21	2.05
Overall	Energy barrier	0.69	1.38
	Reaction energy	1.26	2.05

S2 Related structures of intermolecular interaction

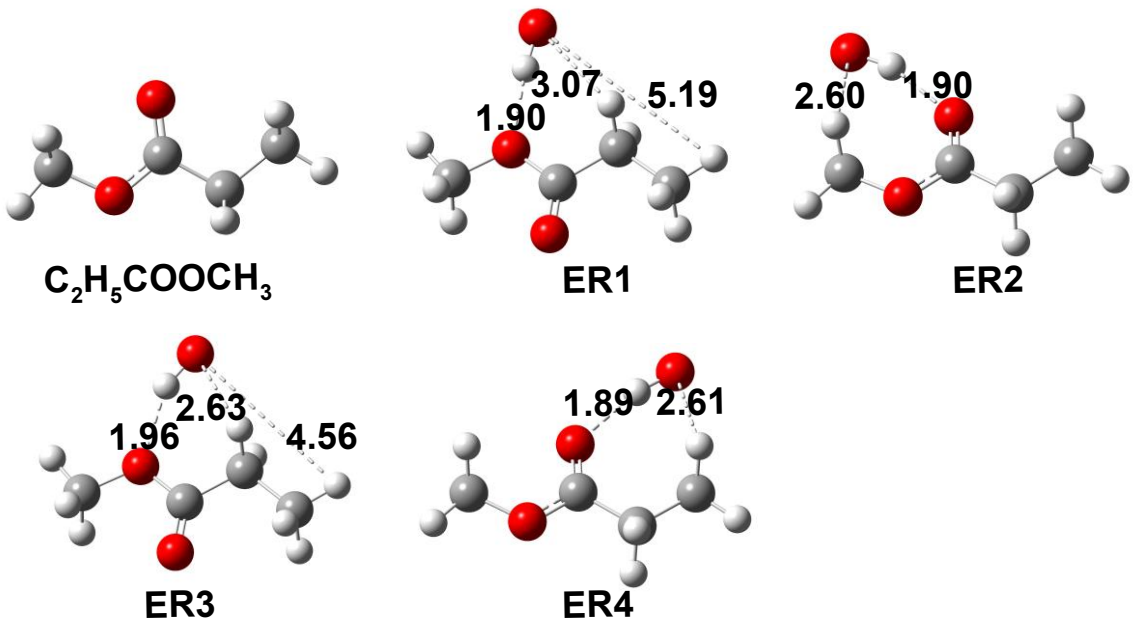

Figure S1. Geometries of the stable structures of $C_2H_5COOCH_3$ and the reactant complexes involved in the reactions of $C_2H_5COOCH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

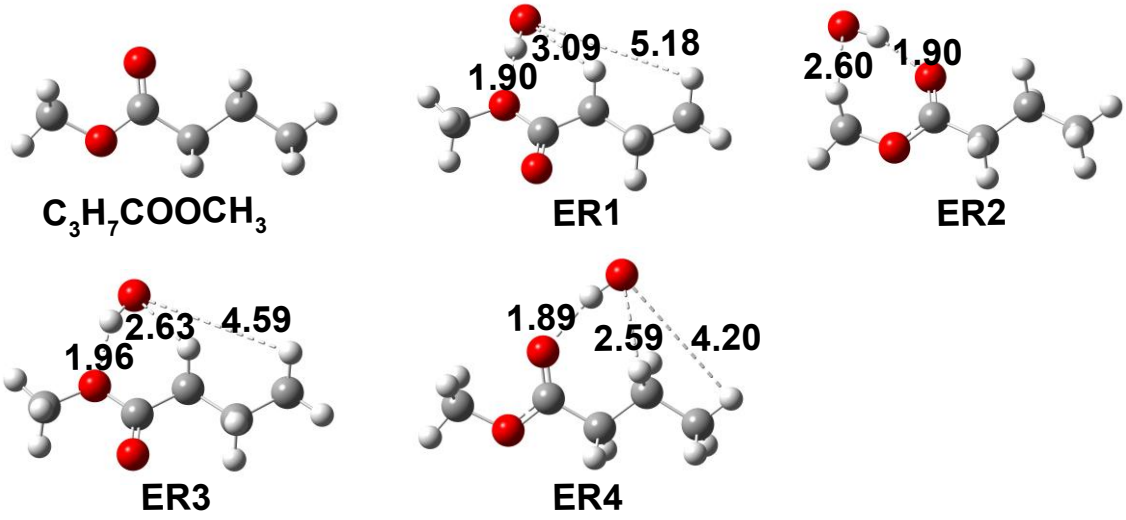

Figure S2. Geometries of the stable structures of $C_3H_7COOCH_3$ and the reactant complexes involved in the reactions of $C_3H_7COOCH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

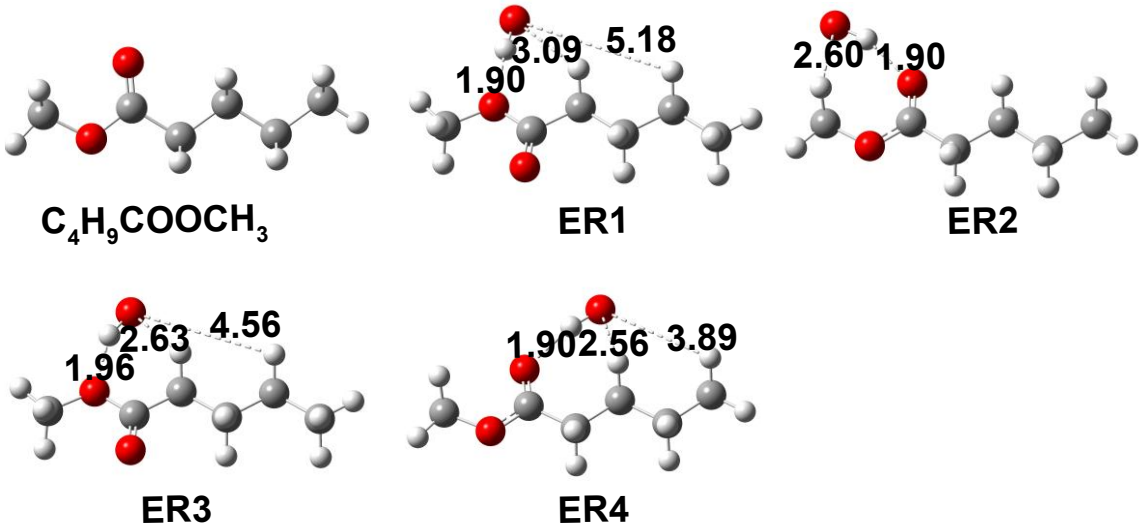

Figure S3. Geometries of the stable structures of $C_4H_9COOCH_3$ and the reactant complexes involved in the reactions of $C_4H_9COOCH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

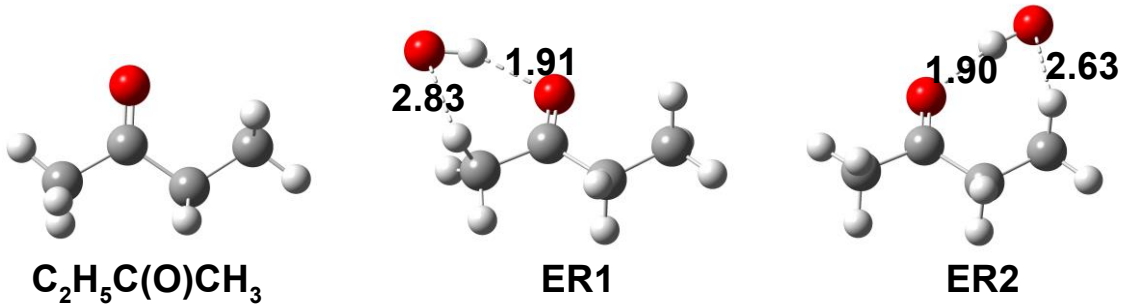

Figure S4. Geometries of the stable structures of $C_2H_5C(O)CH_3$ and the reactant complexes involved in the reactions of $C_2H_5C(O)CH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

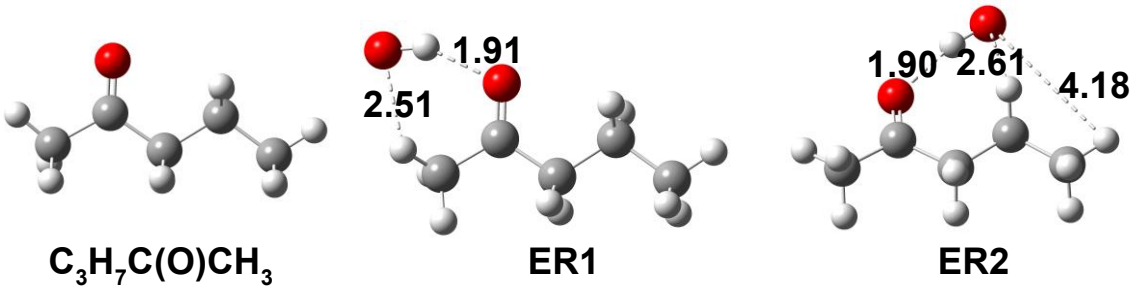

Figure S5. Geometries of the stable structures of $C_3H_7C(O)CH_3$ and the reactant complexes involved in the reactions of $C_3H_7C(O)CH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

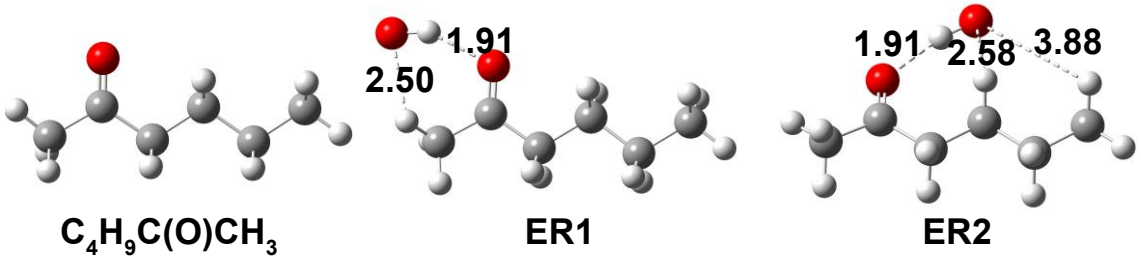

Figure S6. Geometries of the stable structures of $C_4H_9C(O)CH_3$ and the reactant complexes involved in the reactions of $C_4H_9C(O)CH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

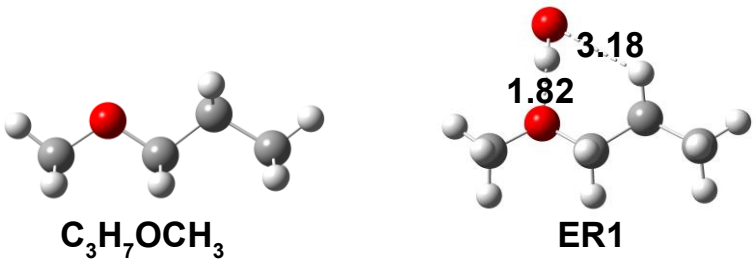

Figure S7. Geometries of the stable structures of $C_3H_7OCH_3$ and the reactant complexes involved in the reactions of $C_3H_7OCH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

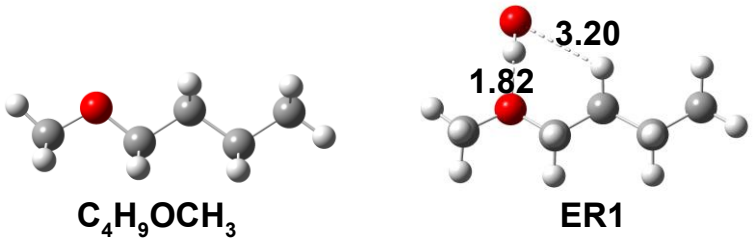

Figure S8. Geometries of the stable structures of $C_4H_9OCH_3$ and the reactant complexes involved in the reactions of $C_4H_9OCH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

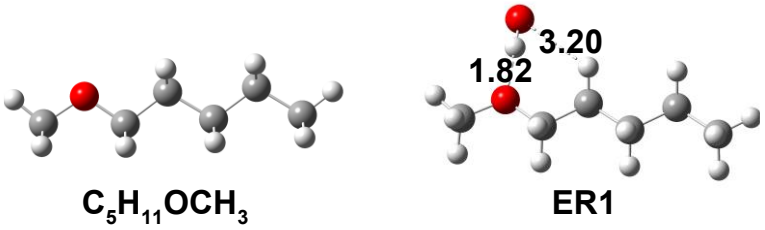

Figure S9. Geometries of the stable structures of $C_5H_{11}OCH_3$ and the reactant complexes involved in the reactions of $C_5H_{11}OCH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

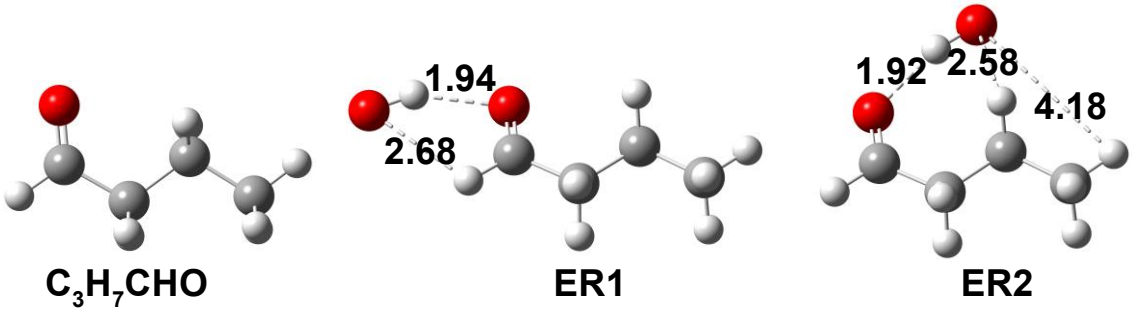

Figure S10. Geometries of the stable structures of C_3H_7CHO and the reactant complexes involved in the reactions of C_3H_7CHO with HȮ optimized at the M06-2X/6-311++G (d, p) level.

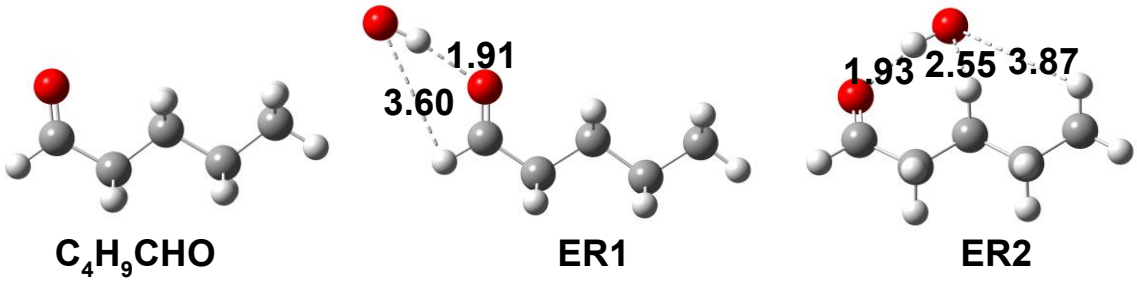

Figure S11. Geometries of the stable structures of C_4H_9CHO and the reactant complexes involved in the reactions of C_4H_9CHO with HȮ optimized at the M06-2X/6-311++G (d, p) level.

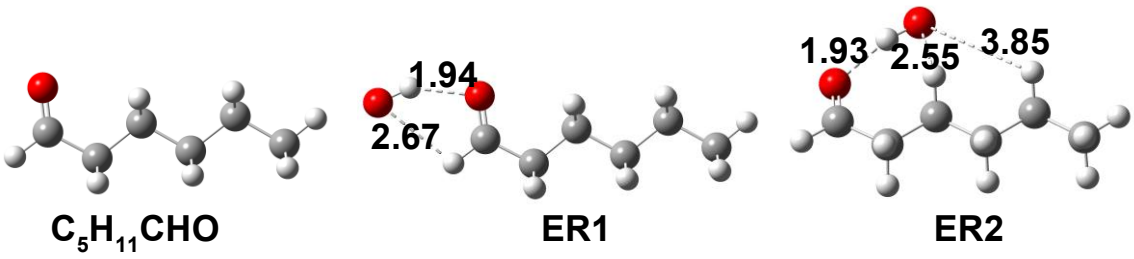

Figure S12. Geometries of the stable structures of $C_5H_{11}CHO$ and the reactant complexes involved in the reactions of $C_5H_{11}CHO$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

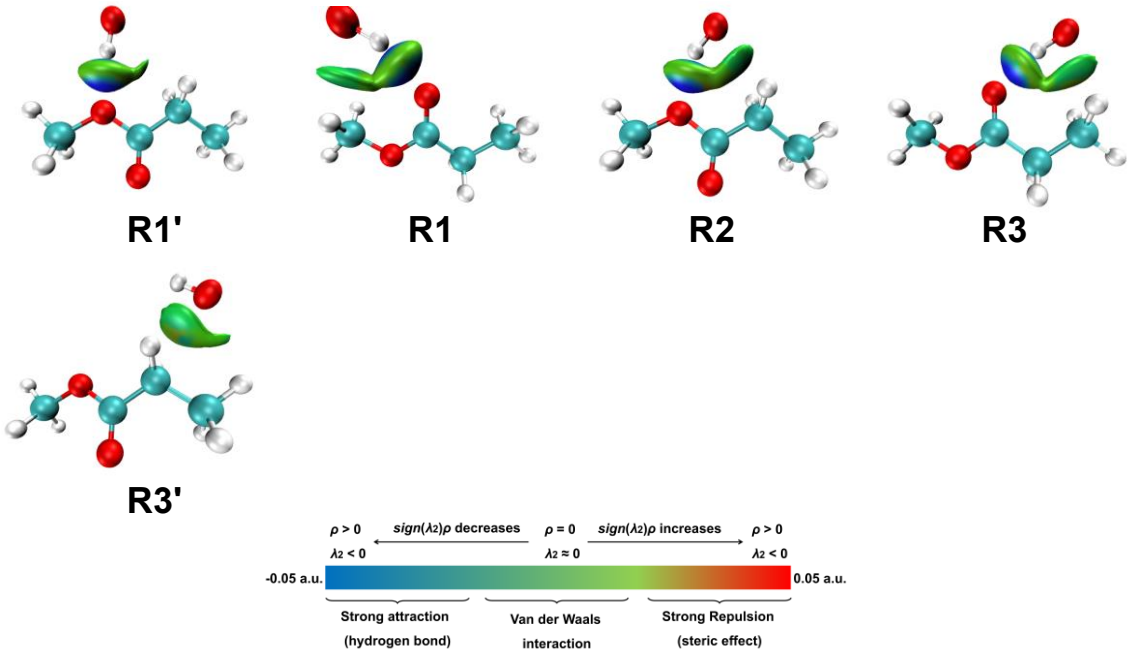

Figure S13. Intermolecular interaction of reactant complexes in the reactions of $CH_3CH_2COOCH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

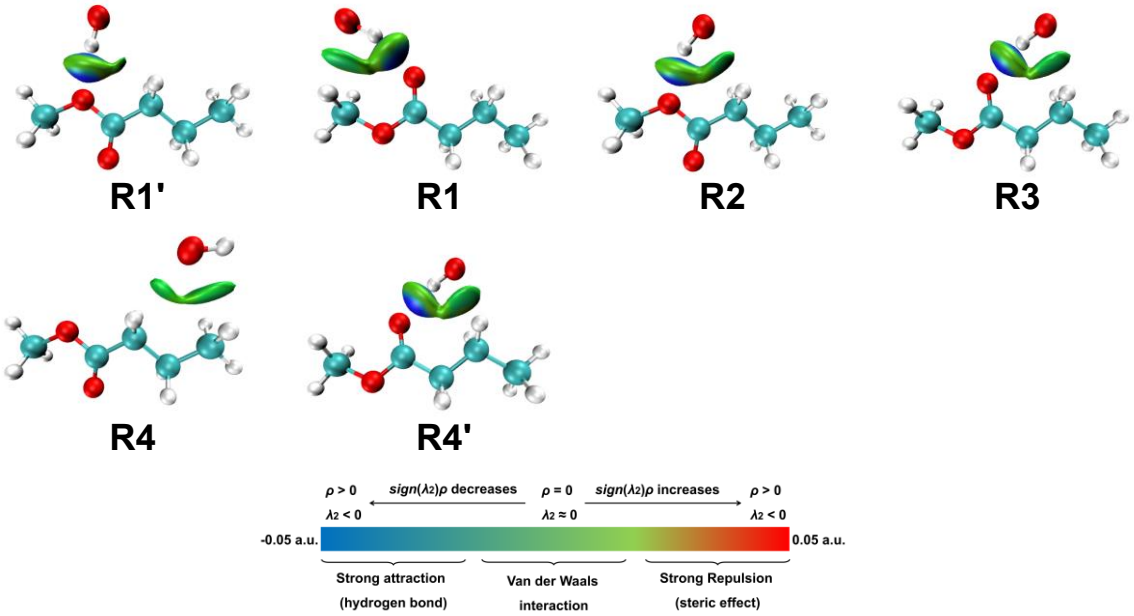

Figure S14. Intermolecular interaction of reactant complexes in the reactions of $CH_3CH_2CH_2COOCH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

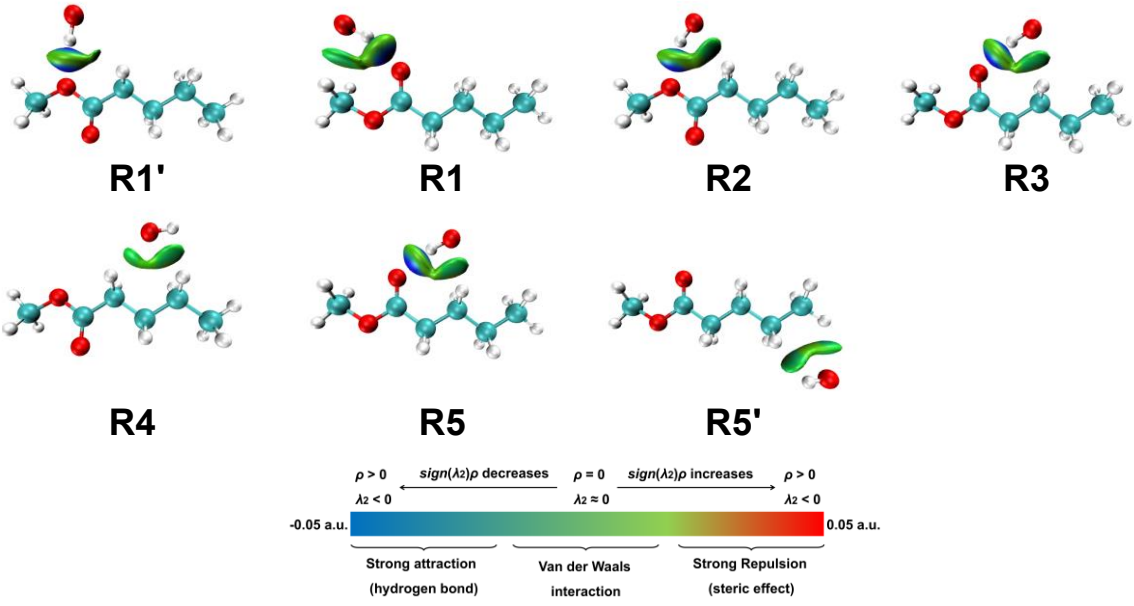

Figure S15. Intermolecular interaction of reactant complexes in the reactions of $CH_3CH_2CH_2CH_2COOCH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

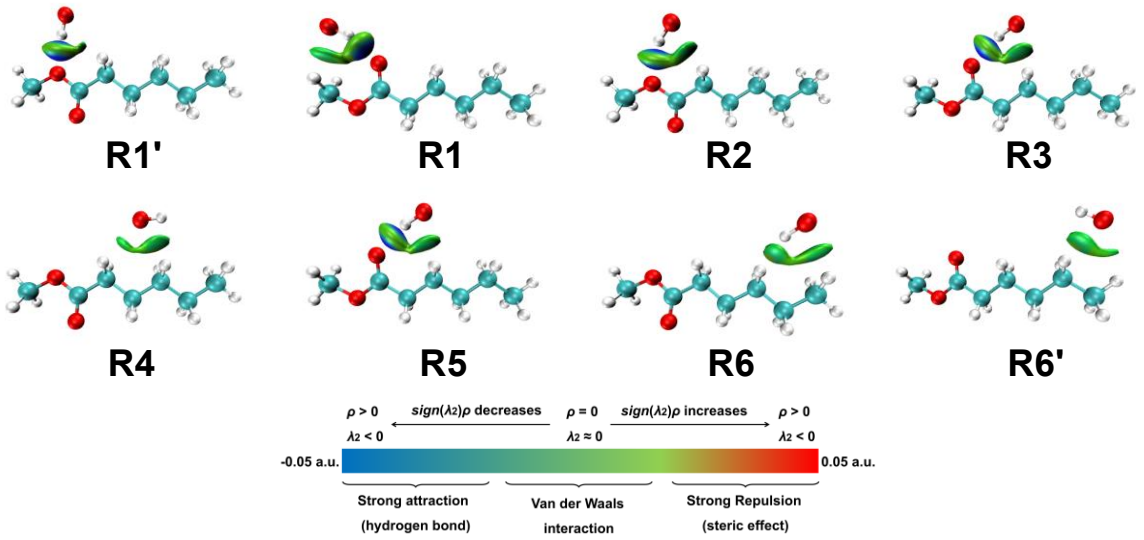

Figure S16. Intermolecular interaction of reactant complexes in the reactions of $CH_3CH_2CH_2CH_2CH_2COOCH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

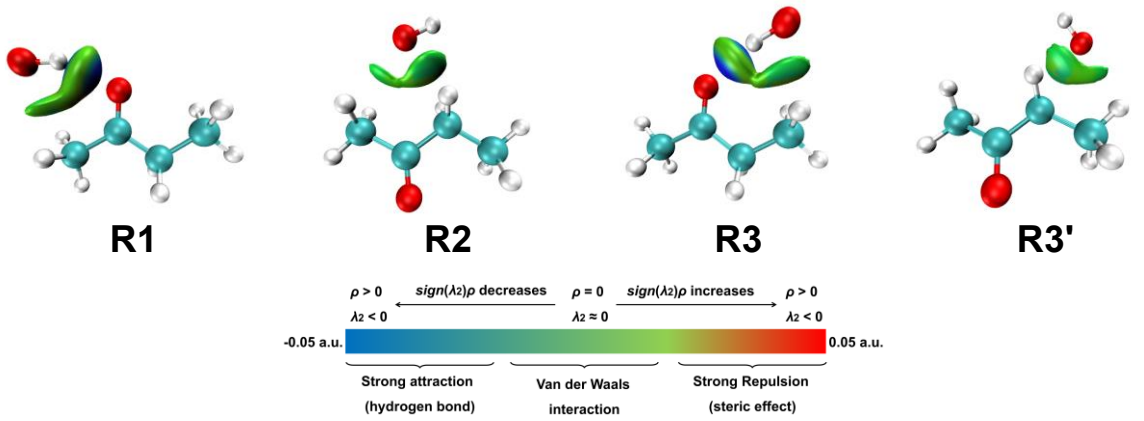

Figure S17. Intermolecular interaction of reactant complexes in the reactions of $CH_3CH_2C(O)CH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

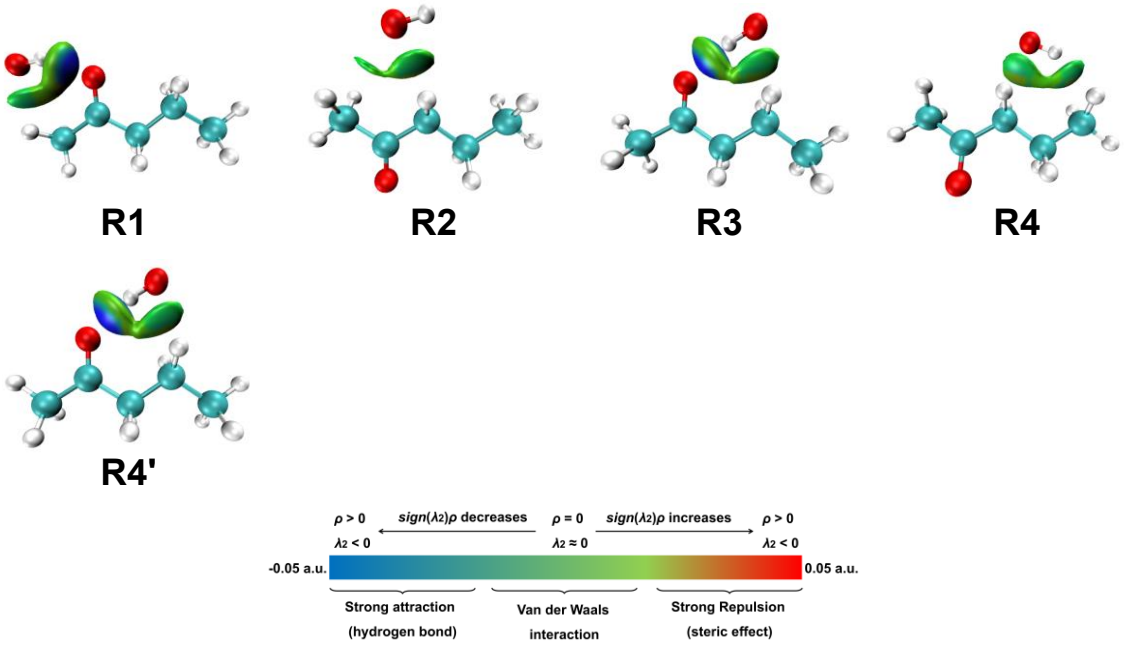

Figure S18. Intermolecular interaction of reactant complexes in the reactions of CH_3CH_2 $CH_2C(O)CH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

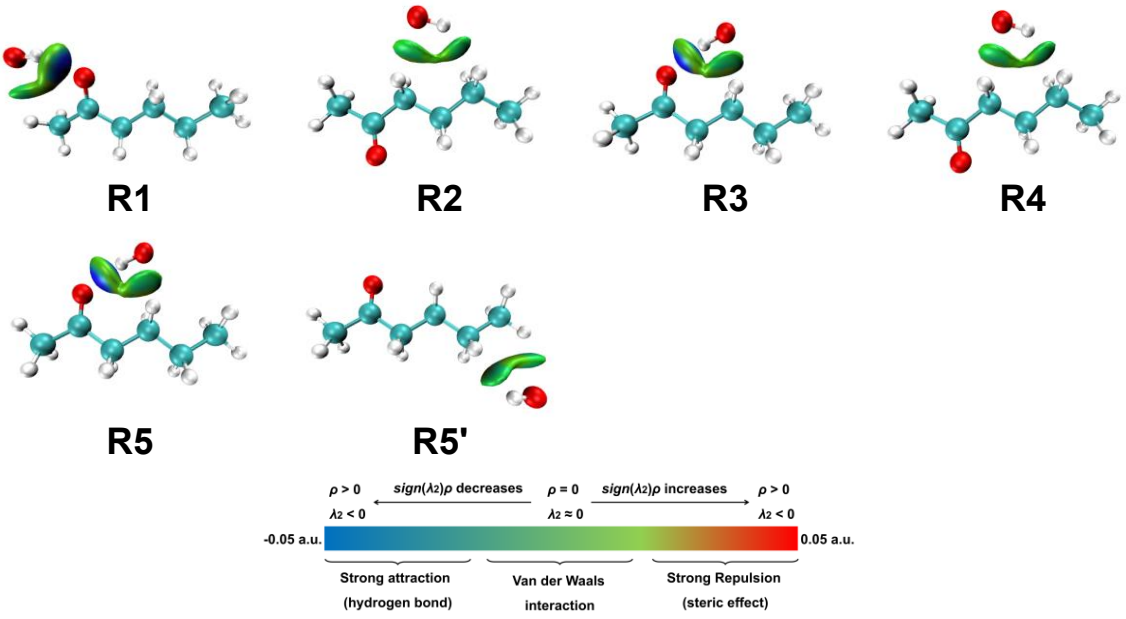

Figure S19. Intermolecular interaction of reactant complexes in the reactions of $CH_3CH_2CH_2$ $CH_2C(O)CH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

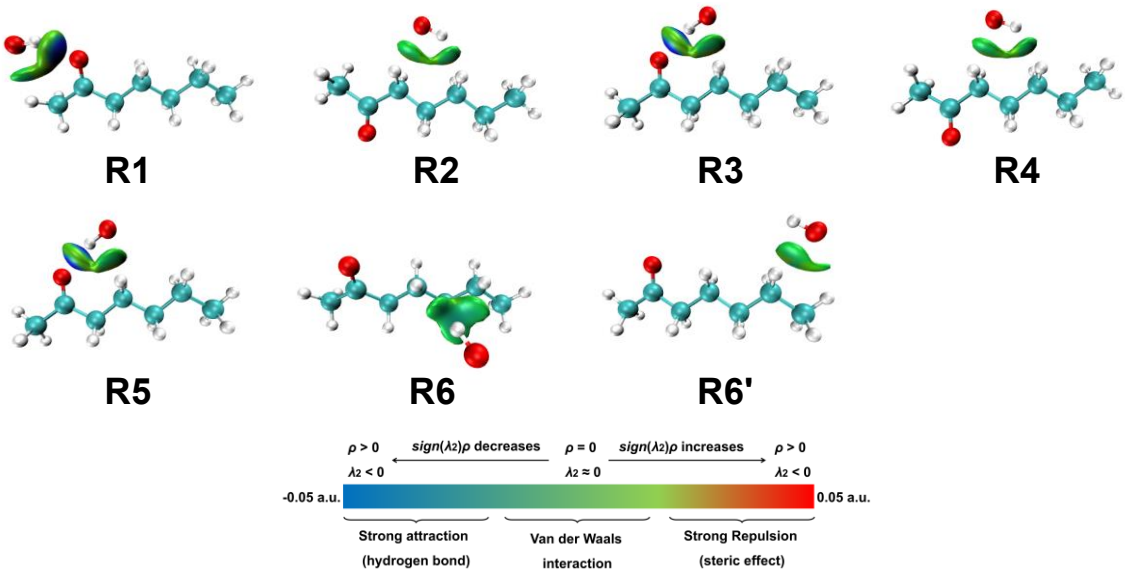

Figure S20. Intermolecular interaction of reactant complexes in the reactions of $CH_3CH_2CH_2CH_2CH_2C(O)CH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

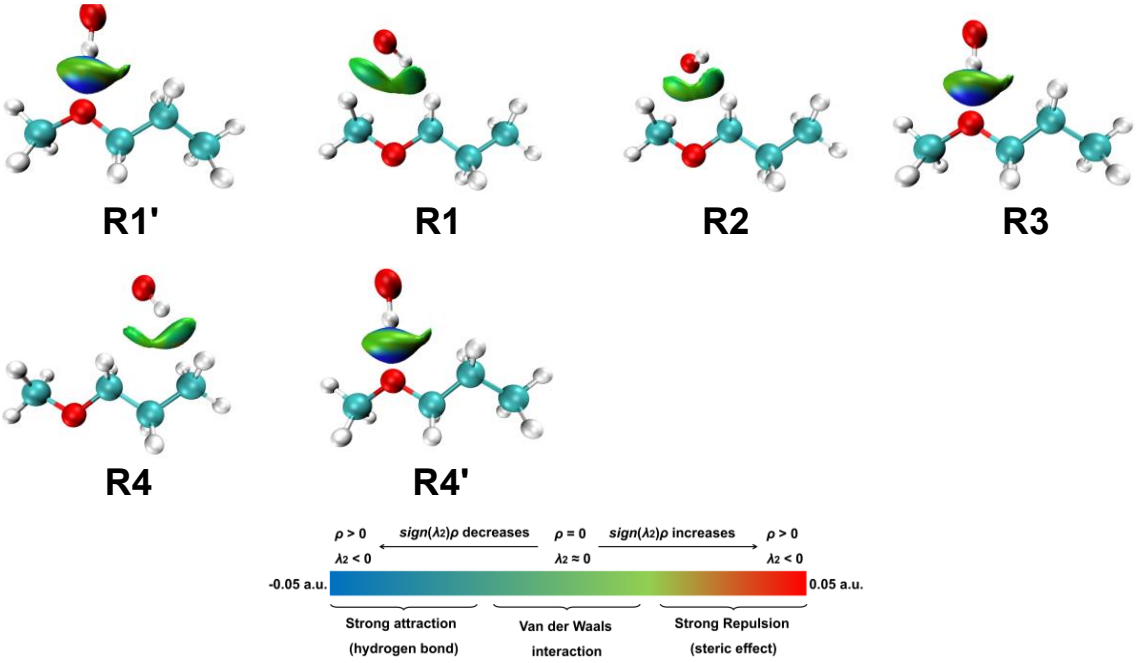

Figure S21. Intermolecular interaction of reactant complexes in the reactions of CH_3CH_2 CH_2OCH_3 with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

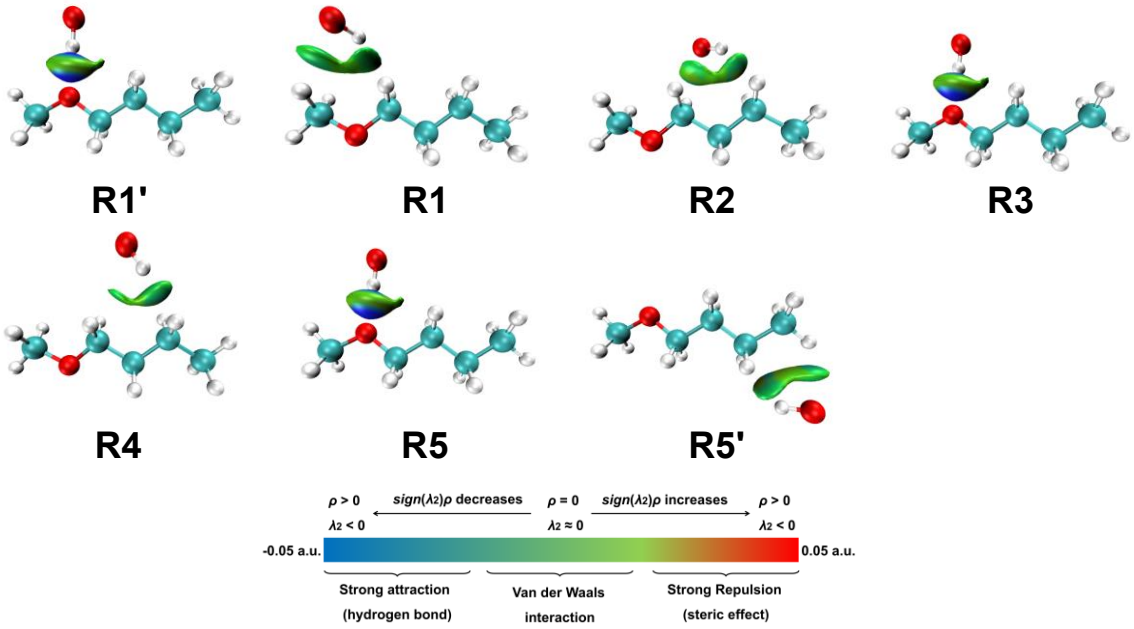

Figure S22. Intermolecular interaction of reactant complexes in the reactions of $CH_3CH_2CH_2$ CH_2OCH_3 with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

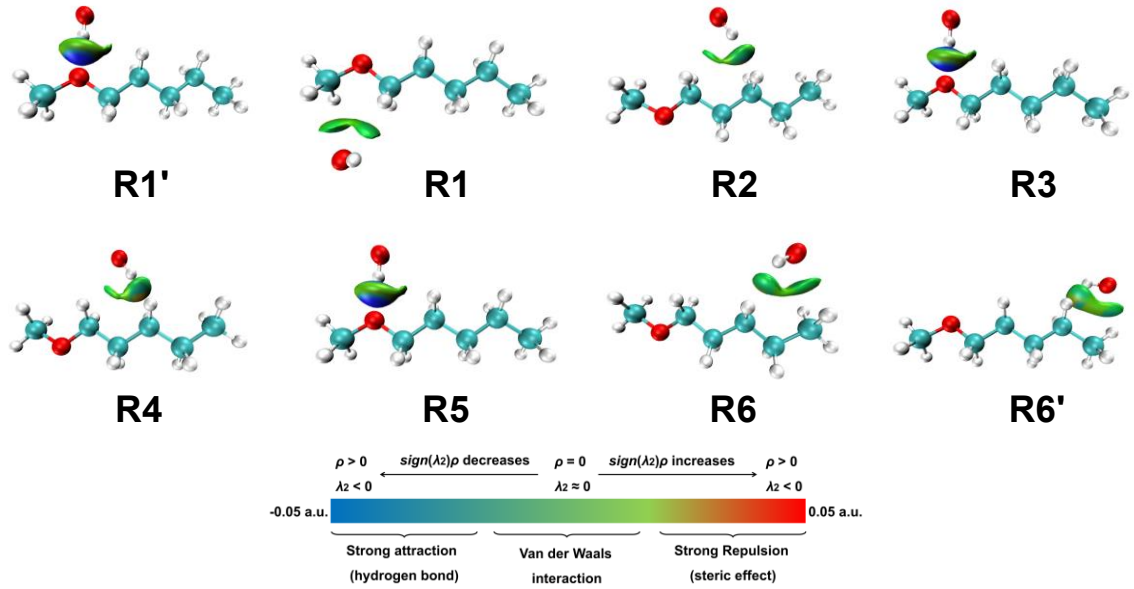

Figure S23. Intermolecular interaction of reactant complexes in the reactions of $CH_3CH_2CH_2$ $CH_2CH_2OCH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

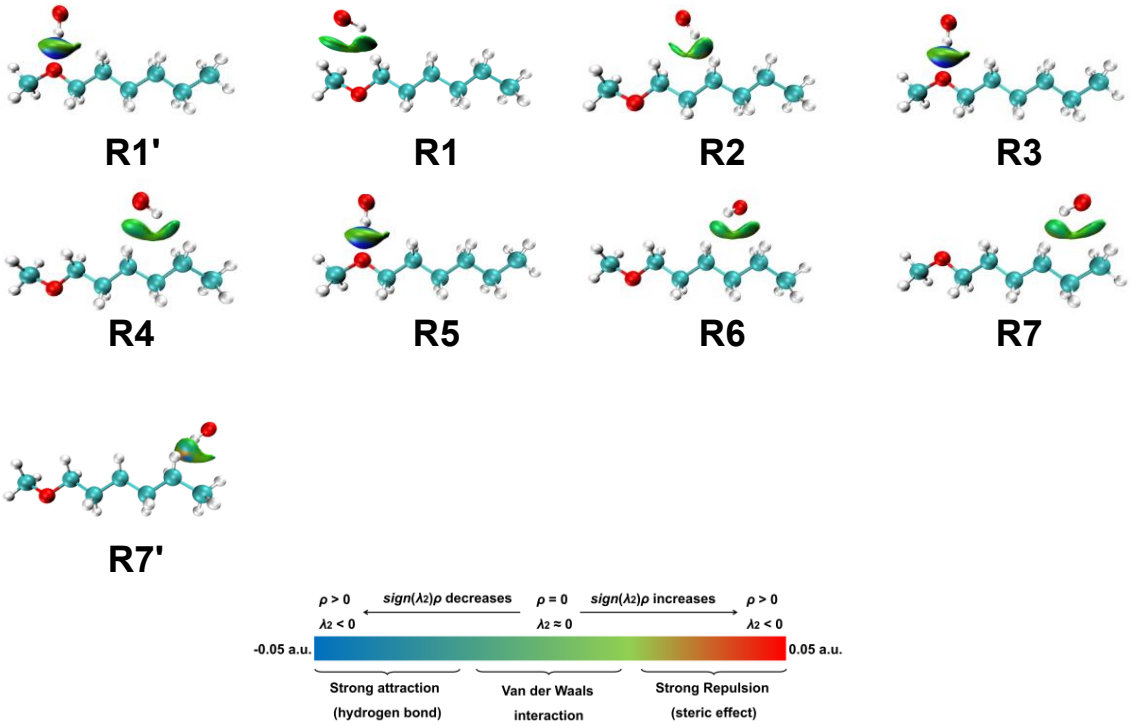

Figure S24. Intermolecular interaction of reactant complexes in the reactions of $CH_3CH_2CH_2CH_2CH_2CH_2OCH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

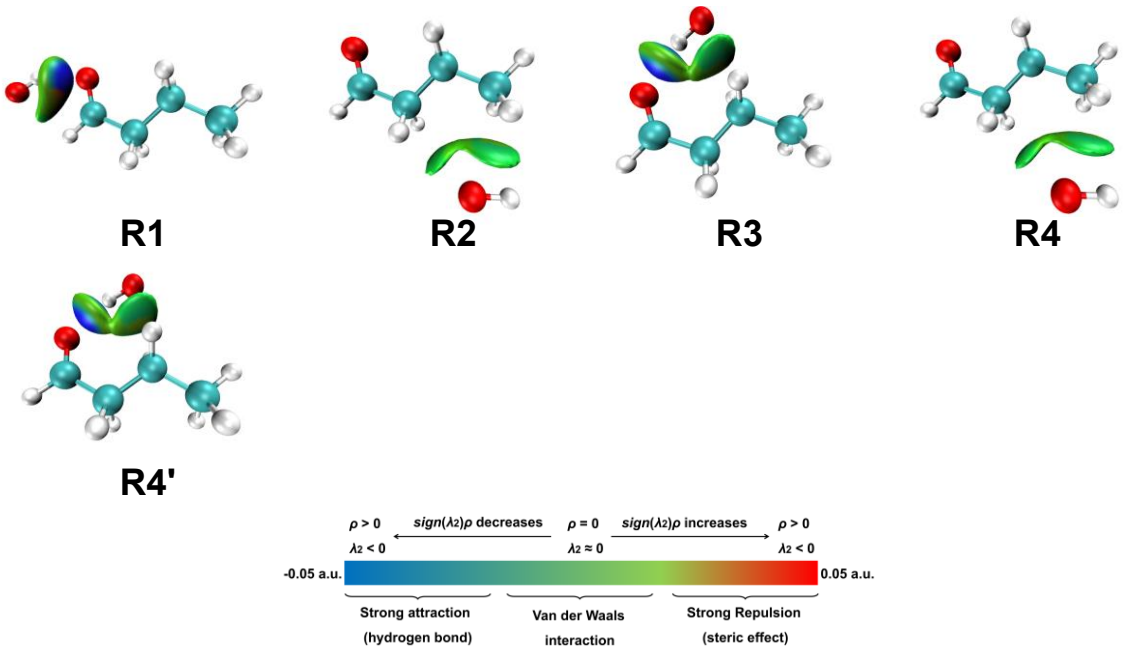

Figure S25. Intermolecular interaction of reactant complexes in the reactions of CH_3 CH_2CH_2CHO with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

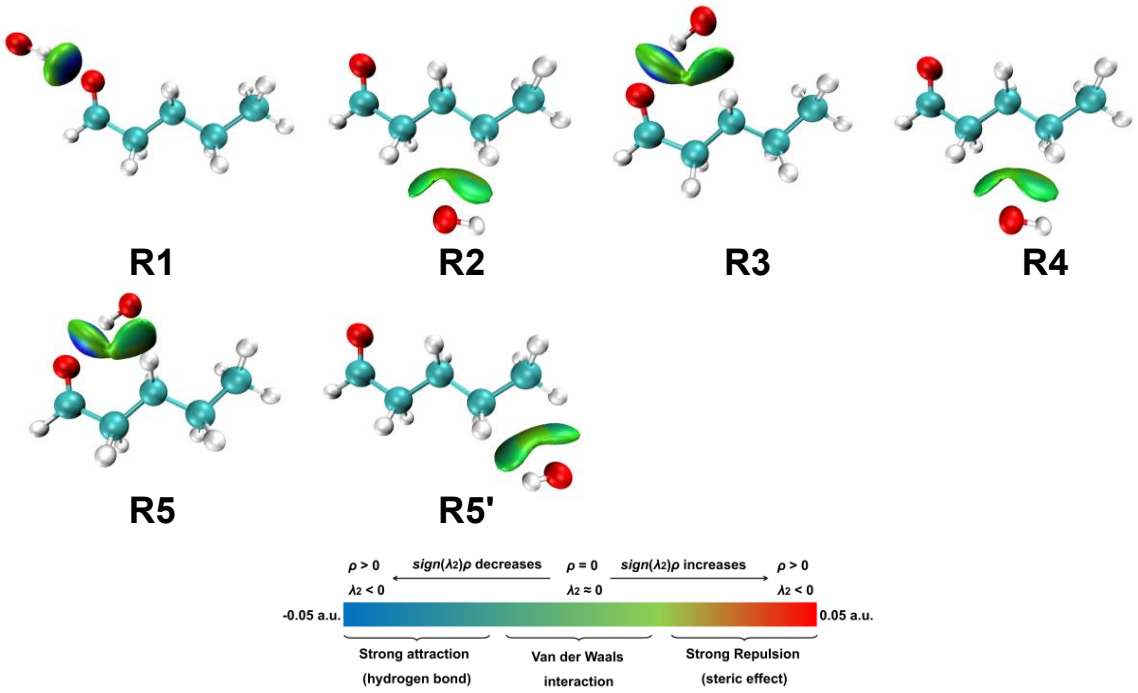

Figure S26. Intermolecular interaction of reactant complexes in the reactions of $CH_3CH_2CH_2CH_2CHO$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

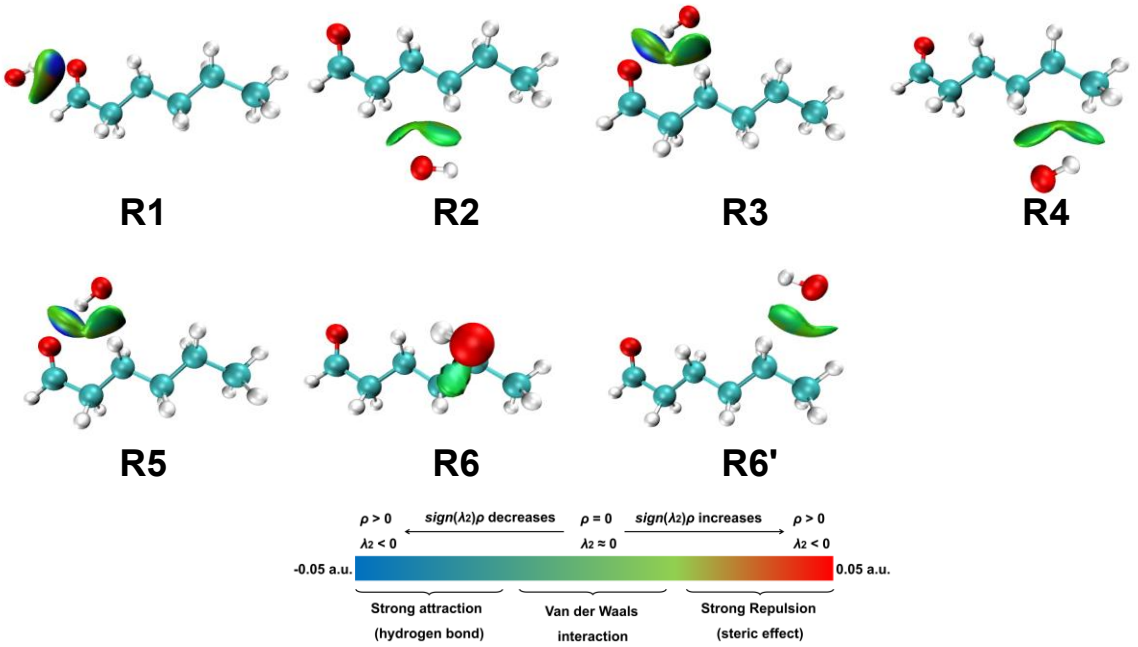

Figure S27. Intermolecular interaction of reactant complexes in the reactions of $CH_3CH_2CH_2CH_2CH_2CHO$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

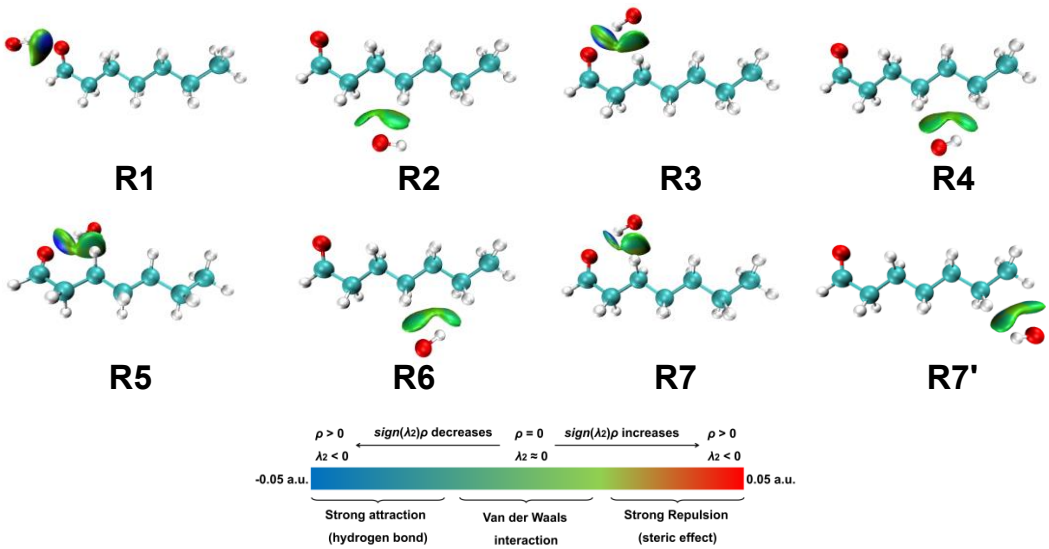

Figure S28. Intermolecular interaction of reactant complexes in the reactions of $CH_3CH_2CH_2CH_2CH_2CH_2CHO$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

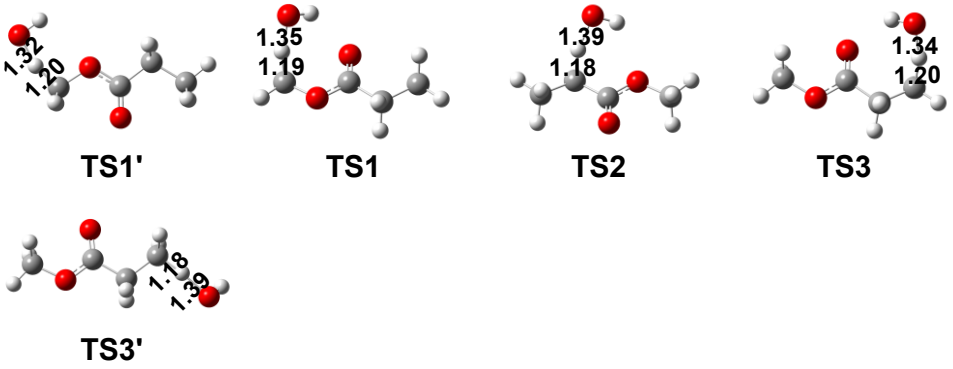

Figure S29. Geometries of the transition states involved in the reactions of $CH_3CH_2COOCH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

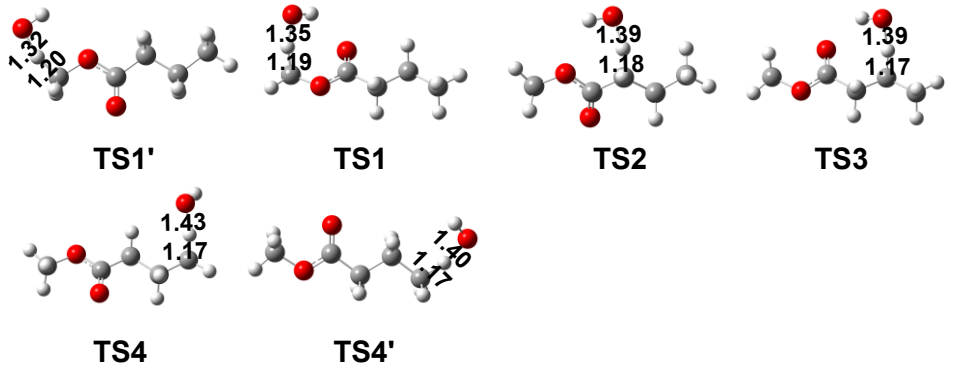

Figure S30. Geometries of the transition states involved in the reactions of $CH_3CH_2CH_2COOCH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

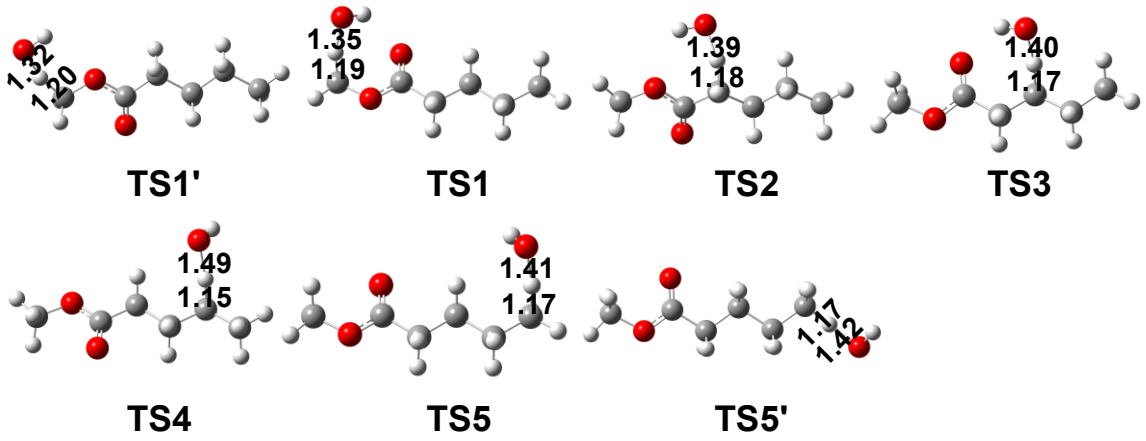

Figure S31. Geometries of the transition states involved in the reactions of $CH_3CH_2CH_2CH_2COOCH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

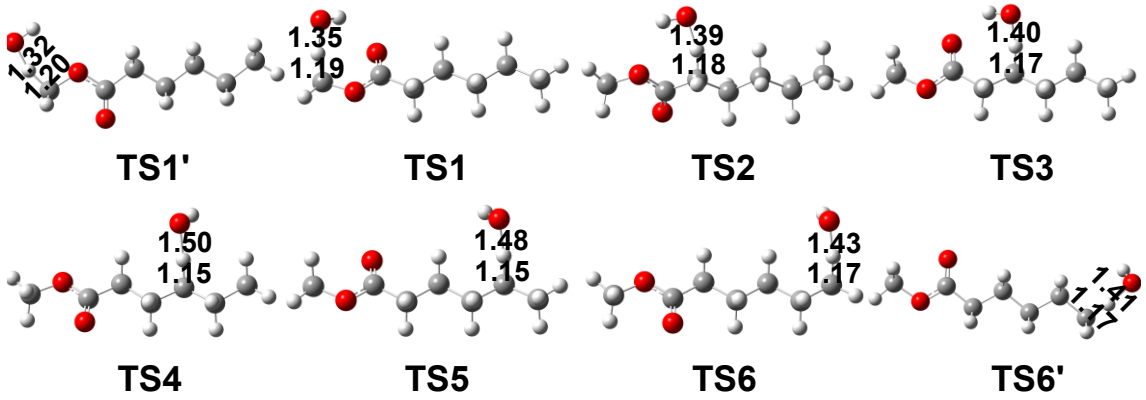

Figure S32. Geometries of the transition states involved in the reactions of $CH_3CH_2CH_2CH_2CH_2COOCH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

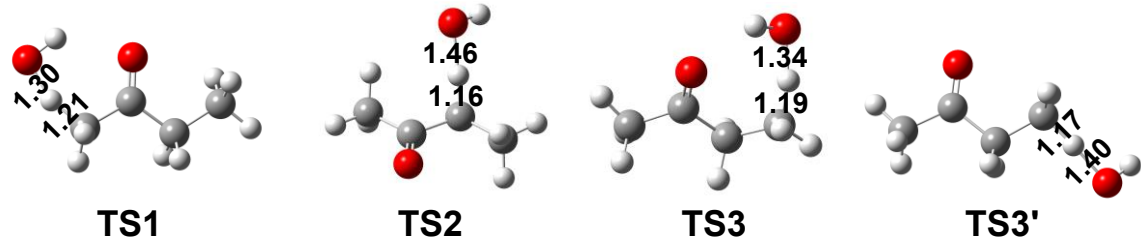

Figure S33. Geometries of the transition states involved in the reactions of $CH_3CH_2C(O)CH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

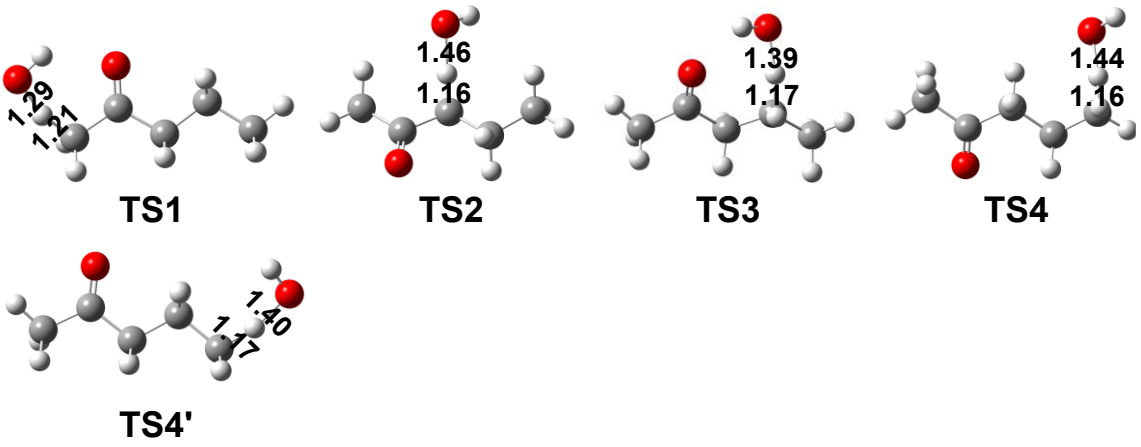

Figure S34. Geometries of the transition states involved in the reactions of $CH_3CH_2CH_2C(O)CH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

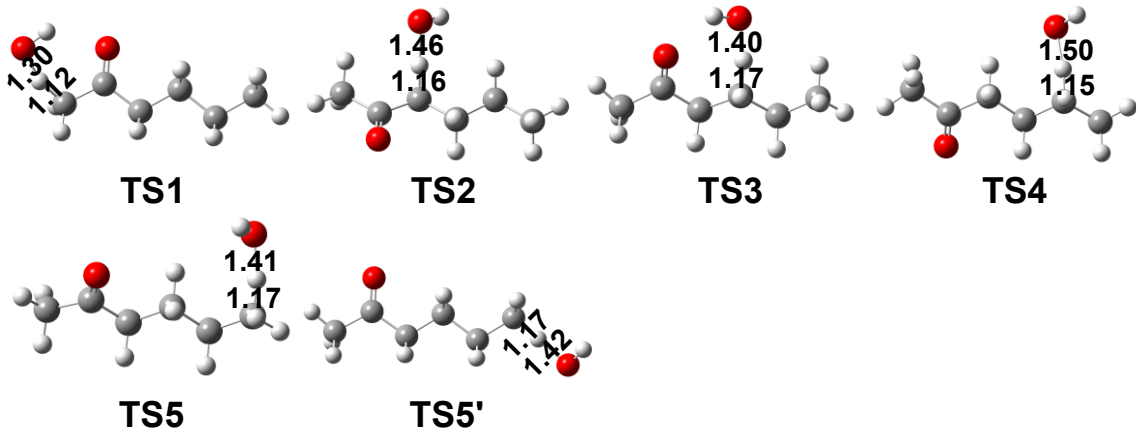

Figure S35. Geometries of the transition states involved in the reactions of $CH_3CH_2CH_2CH_2C(O)CH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

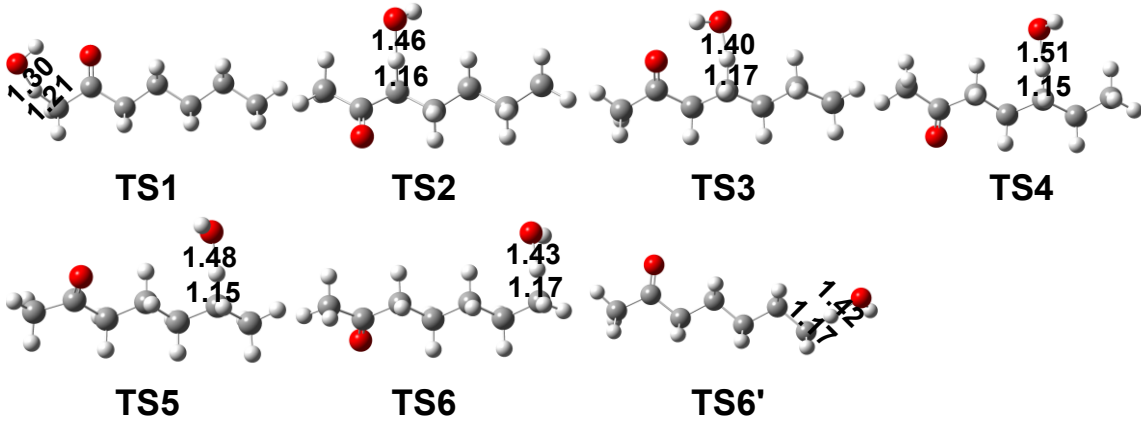

Figure S36. Geometries of the transition states involved in the reactions of $CH_3CH_2CH_2CH_2CH_2C(O)CH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

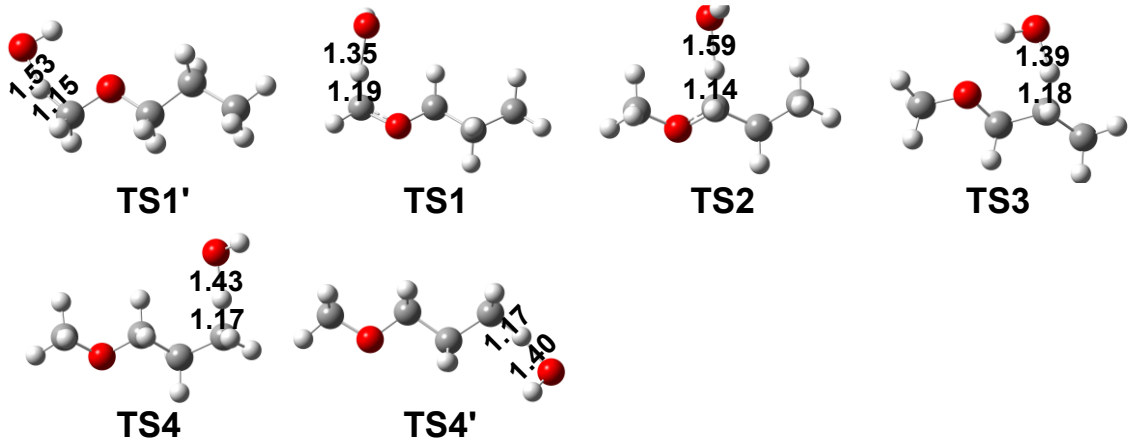

Figure S37. Geometries of the transition states involved in the reactions of $CH_3OCH_2CH_2CH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

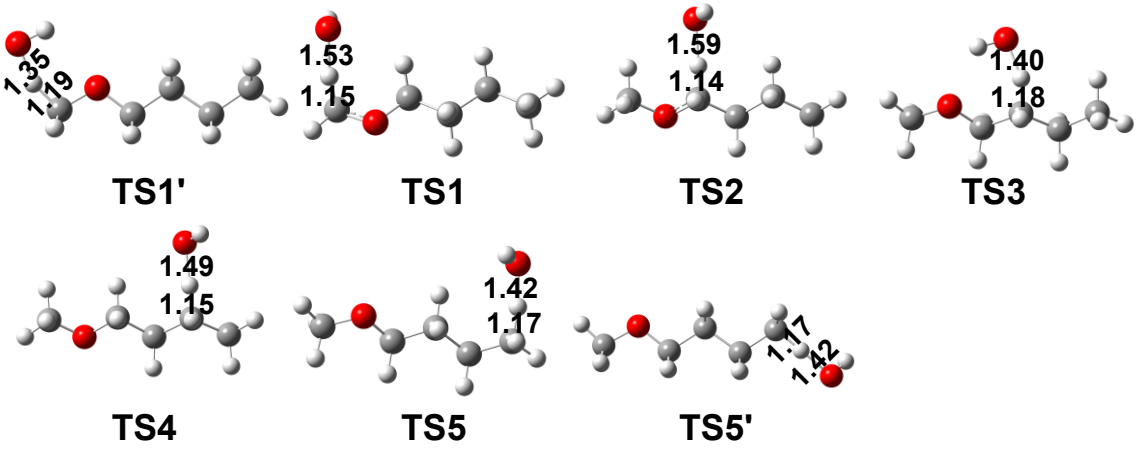

Figure S38. Geometries of the transition states involved in the reactions of $CH_3OCH_2CH_2CH_2CH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

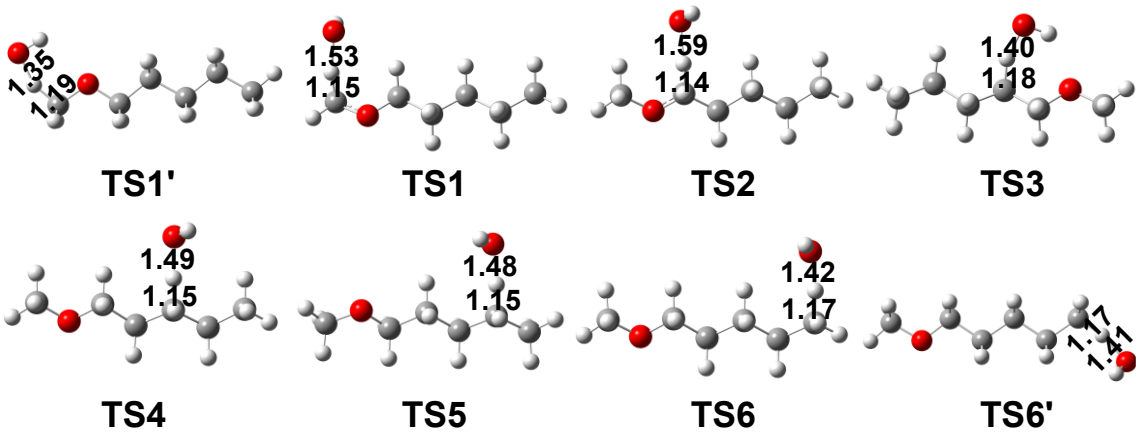

Figure S39. Geometries of the transition states involved in the reactions of $CH_3OCH_2CH_2CH_2CH_2CH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

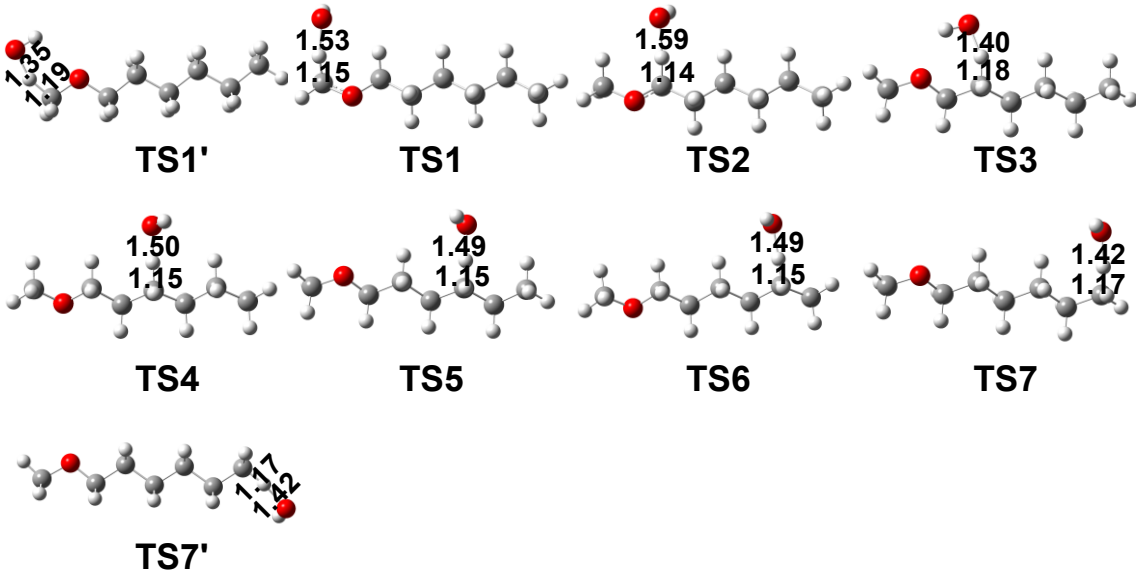

Figure S40. Geometries of the transition states involved in the reactions of $CH_3OCH_2CH_2CH_2CH_2CH_2CH_3$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

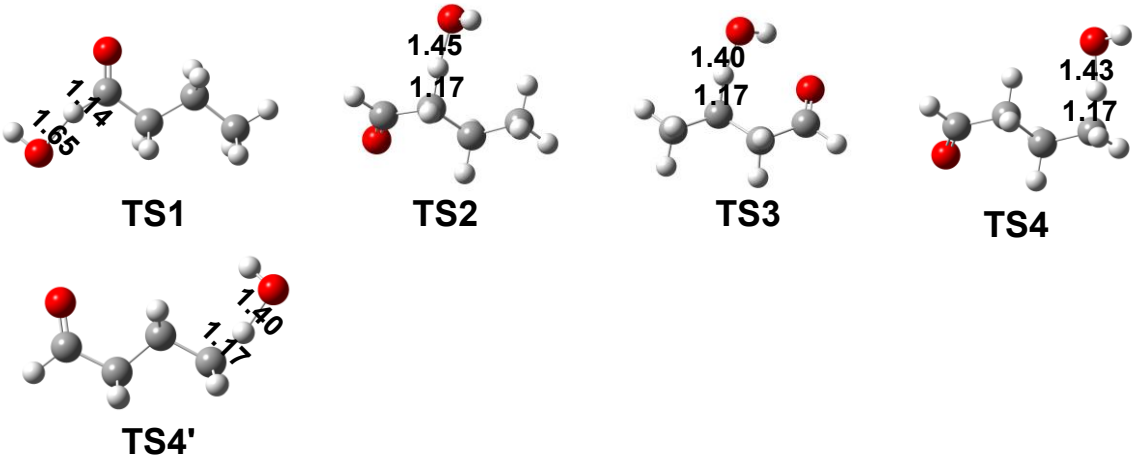

Figure S41. Geometries of the transition states involved in the reactions of $CH_3CH_2CH_2CHO$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

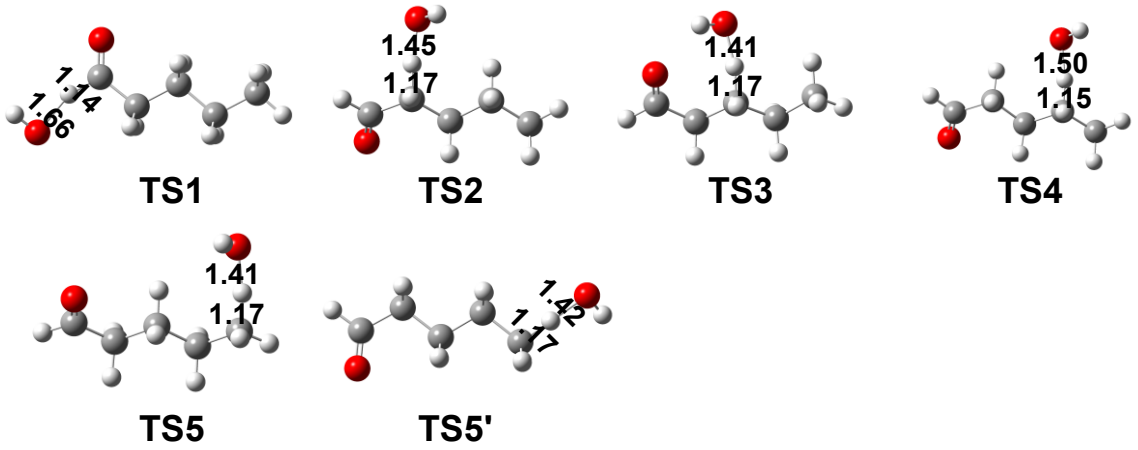

Figure S42. Geometries of the transition states involved in the reactions of $CH_3CH_2CH_2CH_2CHO$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

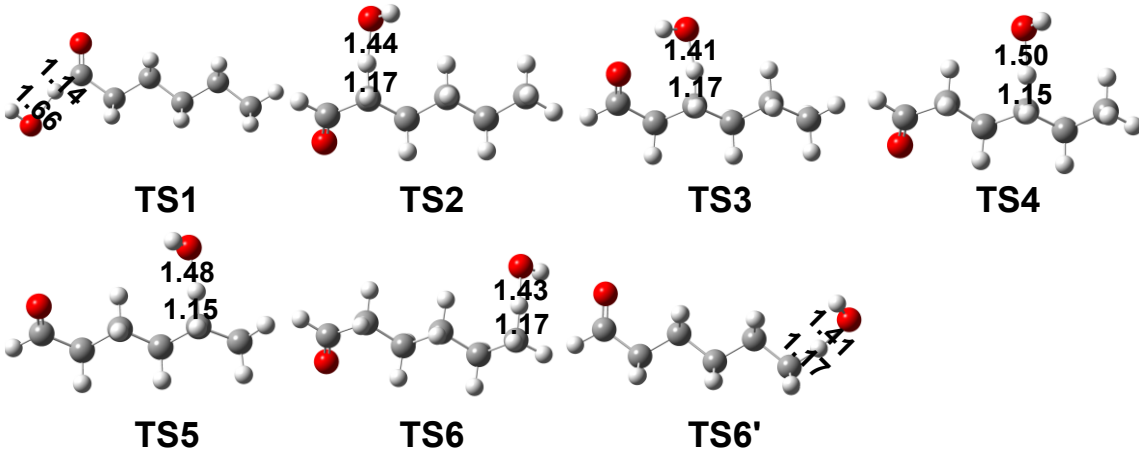

Figure S43. Geometries of the transition states involved in the reactions of $CH_3CH_2CH_2CH_2CH_2CHO$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

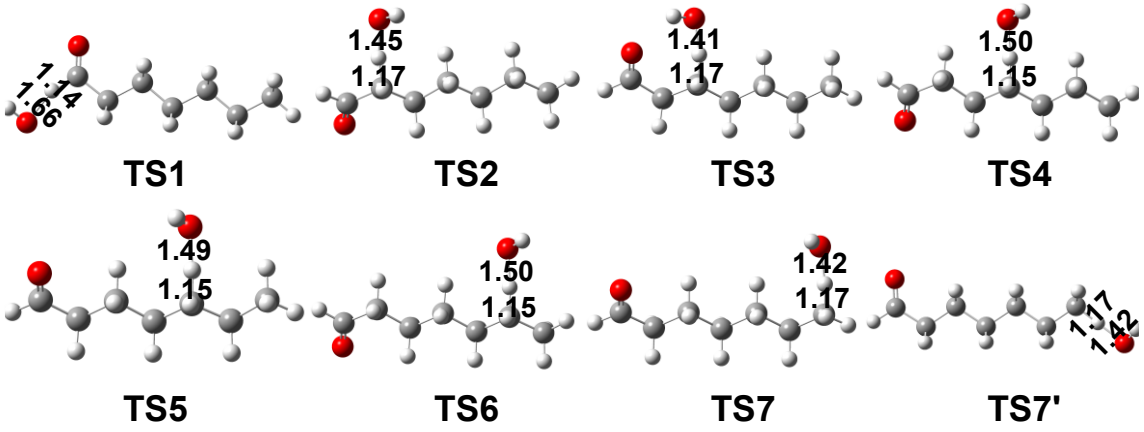

Figure S44. Geometries of the transition states involved in the reactions of $CH_3CH_2CH_2CH_2CH_2CH_2CHO$ with HȮ optimized at the M06-2X/6-311++G (d, p) level.

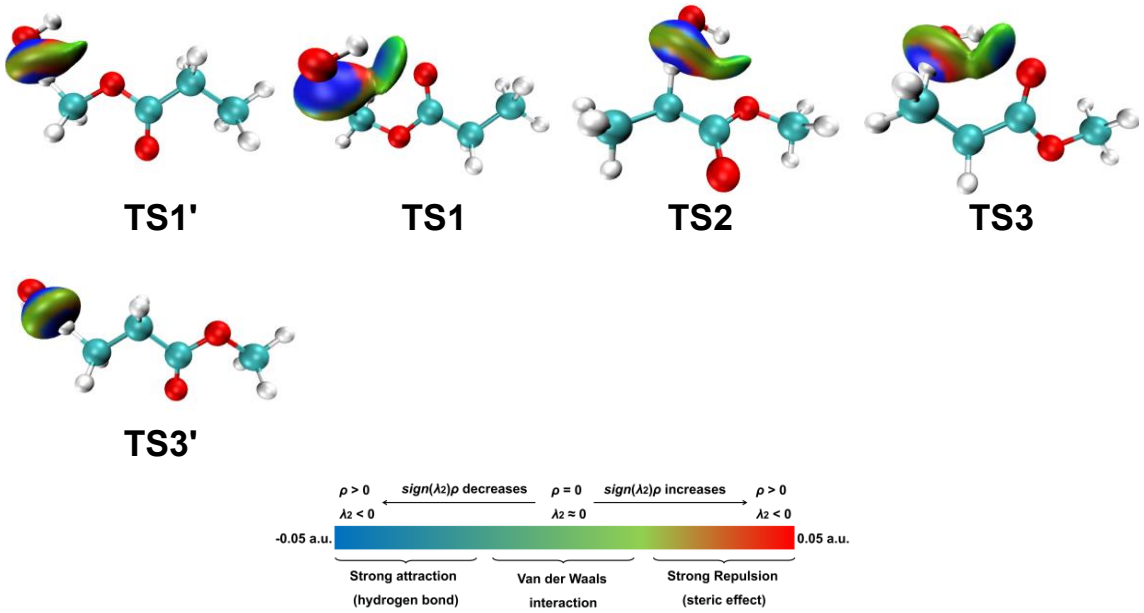

Figure S45. Intermolecular interaction of transition states in the reactions of $CH_3CH_2COOCH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

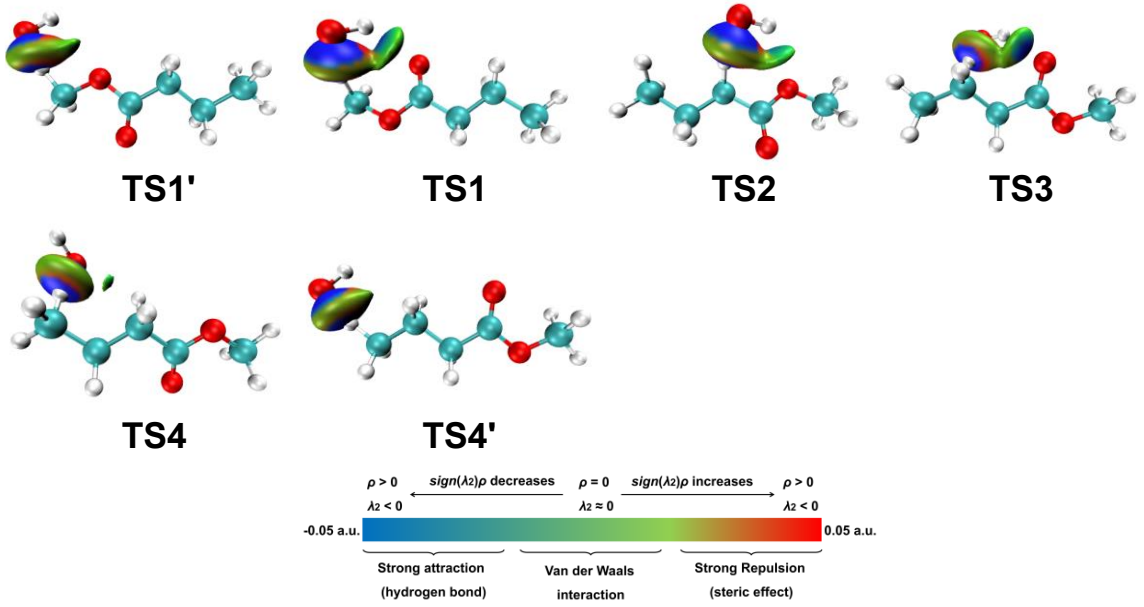

Figure S46. Intermolecular interaction of transition states in the reactions of $CH_3CH_2CH_2COOCH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

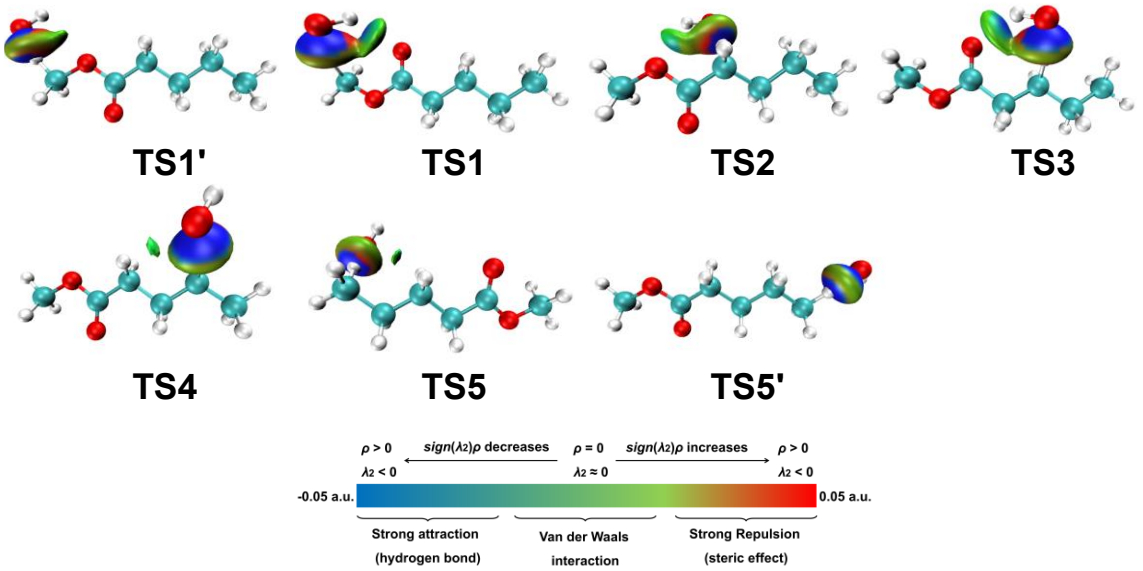

Figure S47. Intermolecular interaction of transition states in the reactions of $CH_3CH_2CH_2CH_2COOCH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

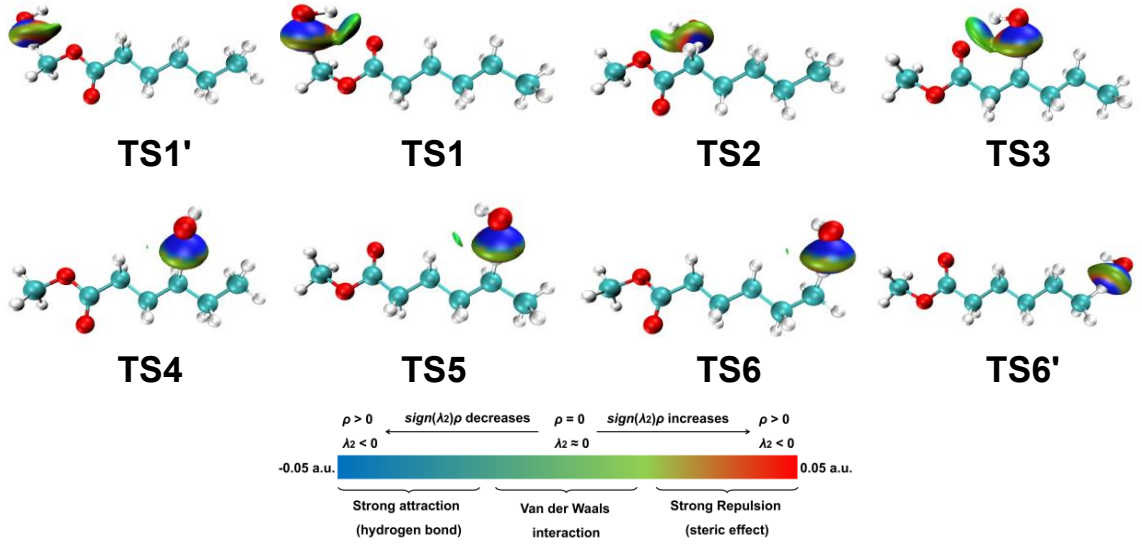

Figure S48. Intermolecular interaction of transition states in the reactions of $CH_3CH_2CH_2CH_2CH_2COOCH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

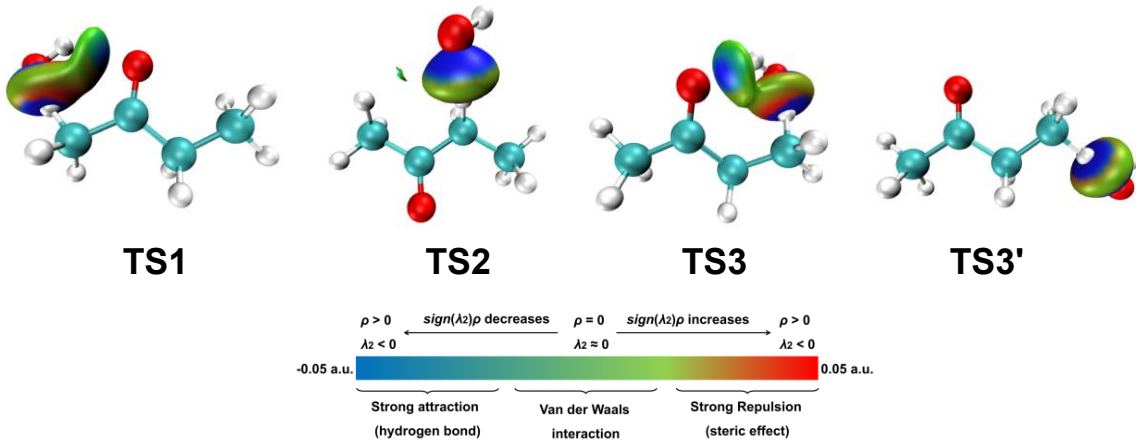

Figure S49. Intermolecular interaction of transition states in the reactions of $CH_3CH_2C(O)CH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

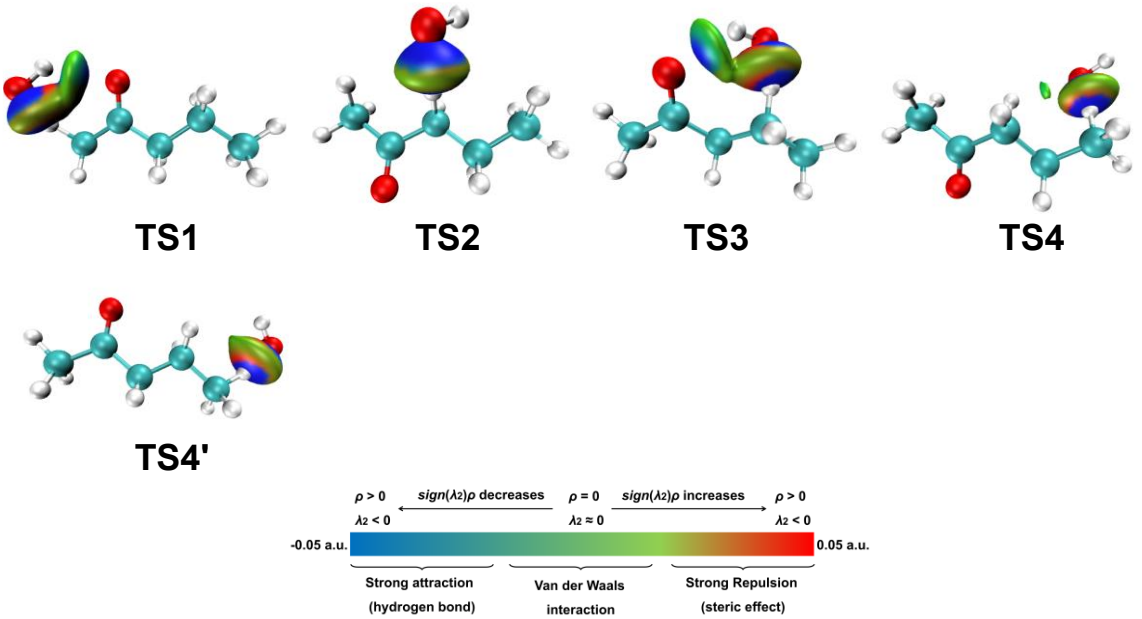

Figure S50. Intermolecular interaction of transition states in the reactions of CH_3CH_2 $CH_2C(O)CH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

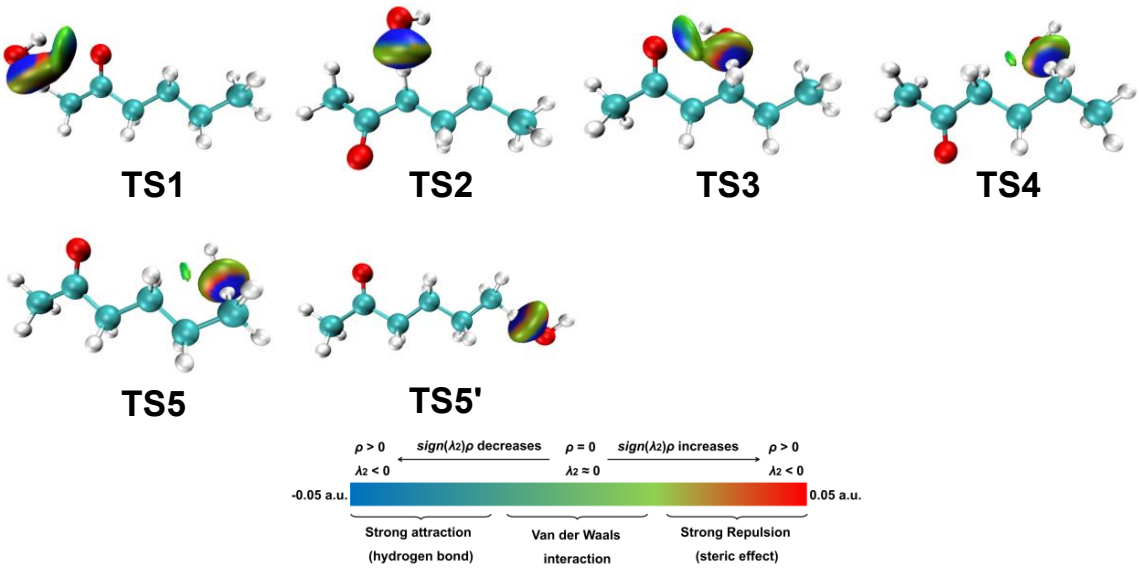

Figure S51. Intermolecular interaction of transition states in the reactions of $CH_3CH_2CH_2$ $CH_2C(O)CH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

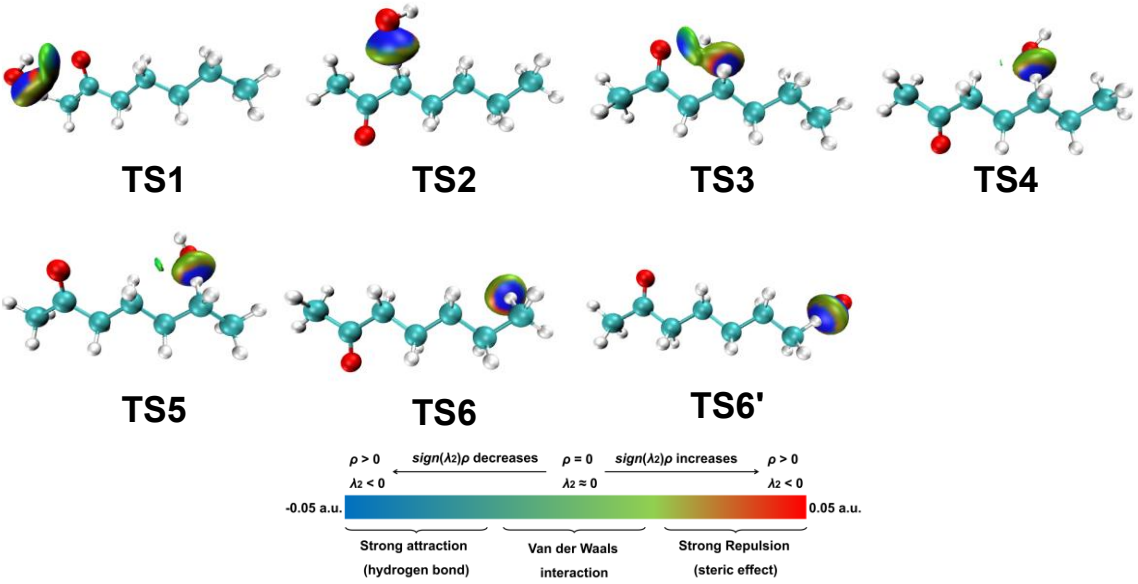

Figure S52. Intermolecular interaction of transition states in the reactions of $CH_3CH_2CH_2CH_2$ $CH_2C(O)CH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

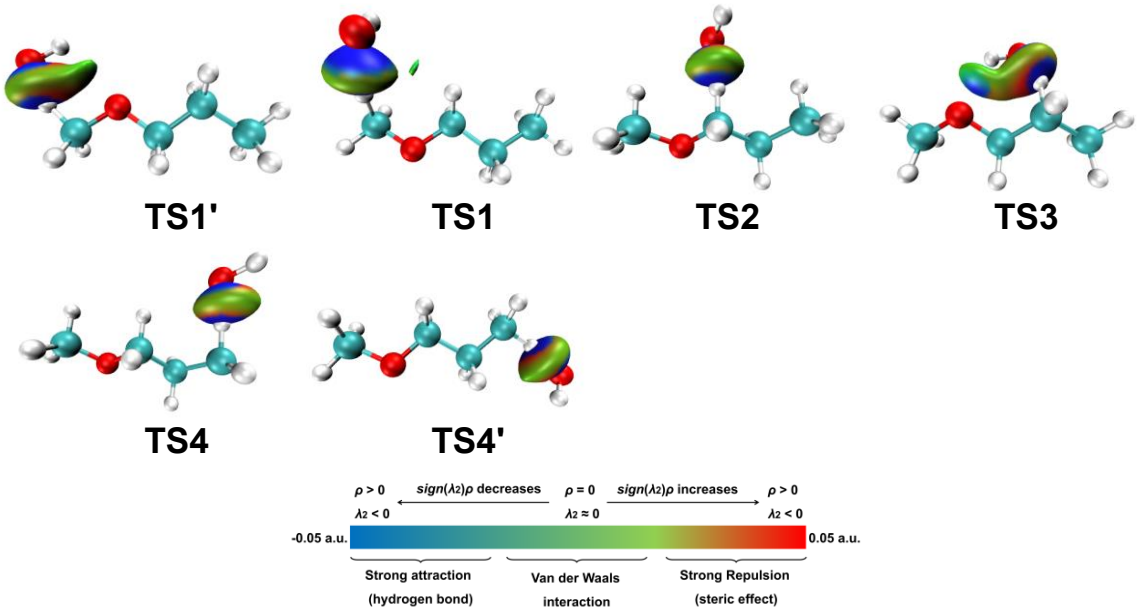

Figure S53. Intermolecular interaction of transition states in the reactions of $CH_3OCH_2CH_2CH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

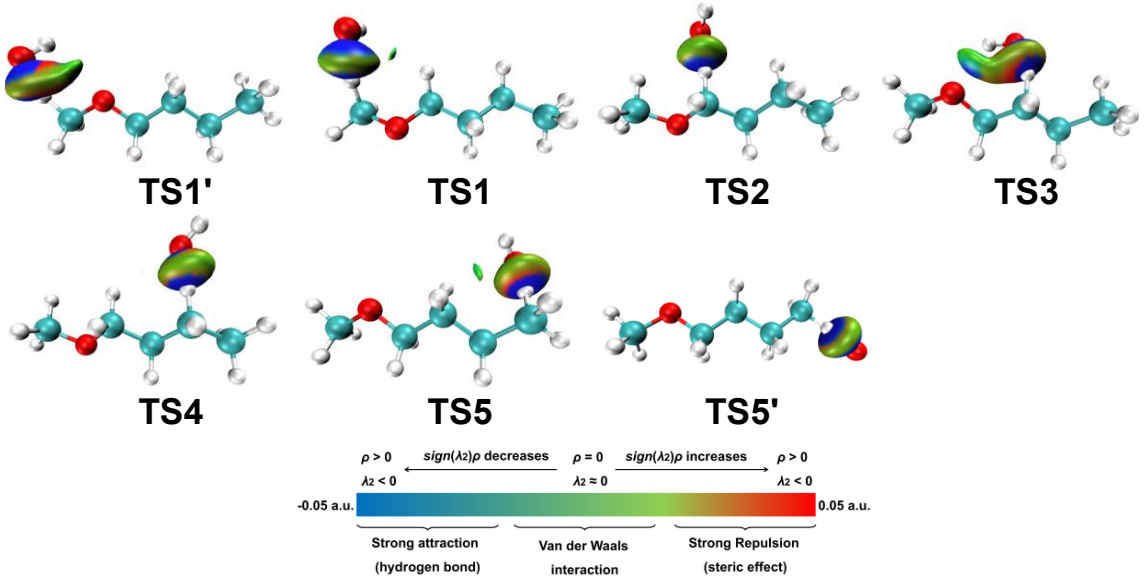

Figure S54. Intermolecular interaction of transition states in the reactions of $CH_3OCH_2CH_2CH_2CH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

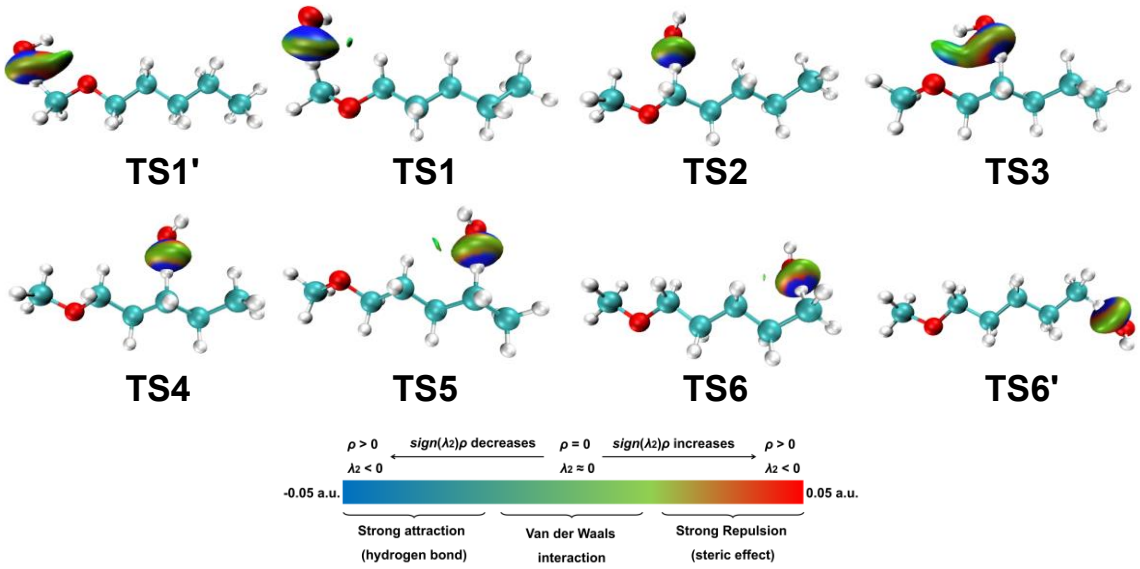

Figure S55. Intermolecular interaction of transition states in the reactions of $CH_3OCH_2CH_2CH_2CH_2CH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

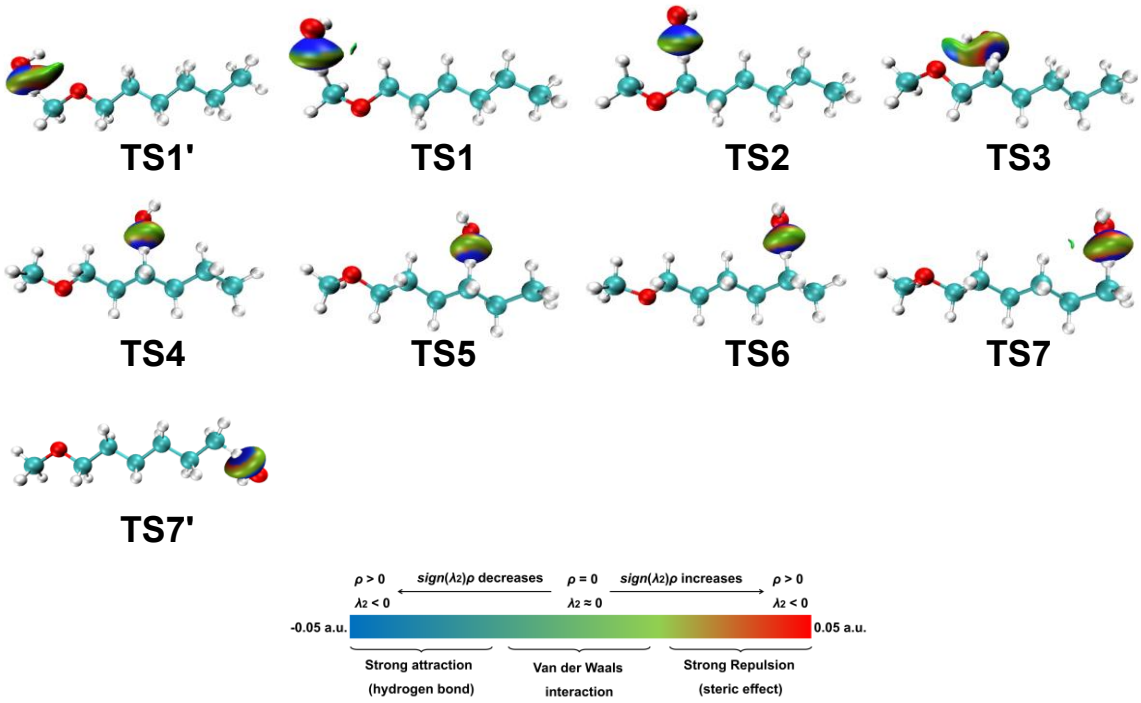

Figure S56. Intermolecular interaction of transition states in the reactions of $CH_3OCH_2CH_2CH_2CH_2CH_2CH_3$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

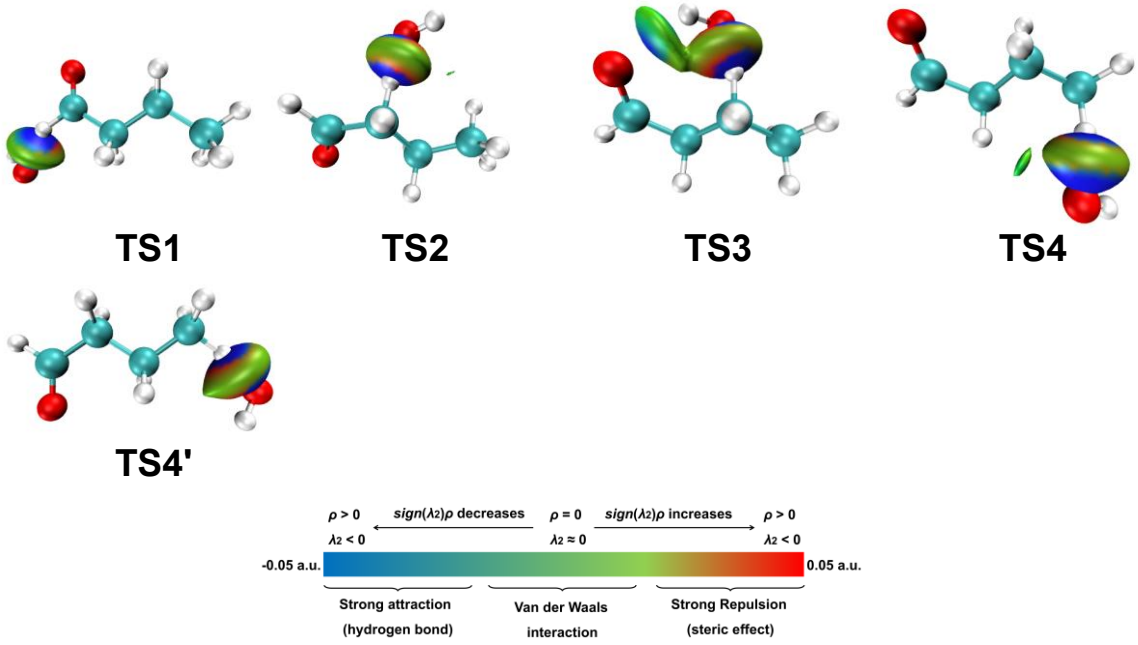

Figure S57. Intermolecular interaction of transition states in the reactions of $CH_3CH_2CH_2CHO$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

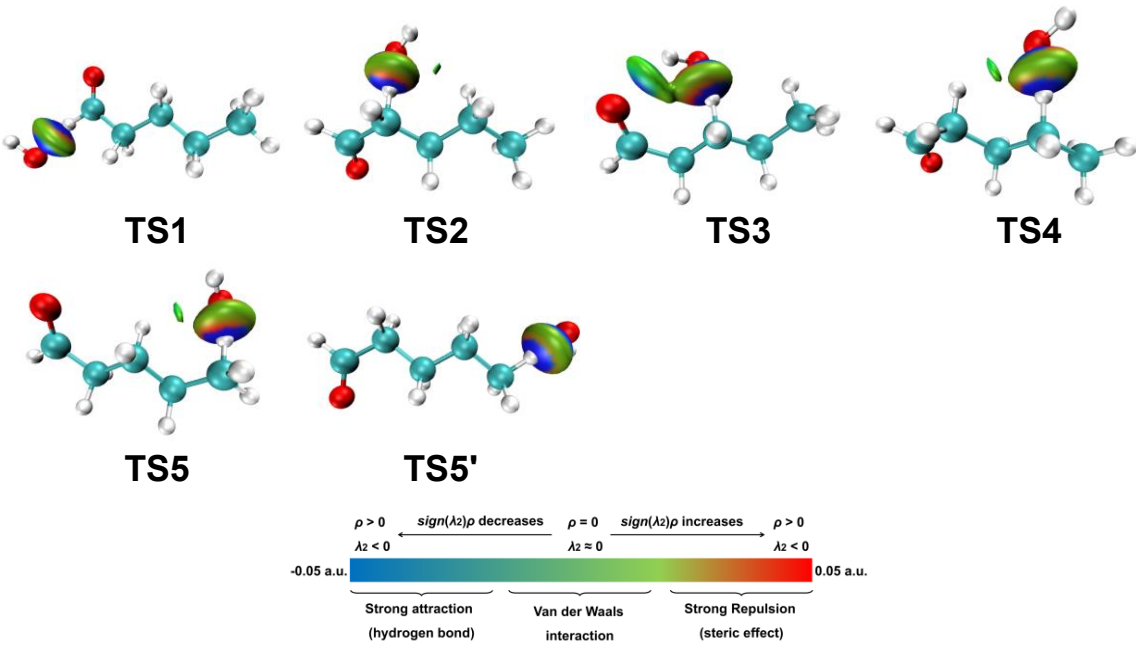

Figure S58. Intermolecular interaction of transition states in the reactions of $CH_3CH_2CH_2CH_2CHO$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

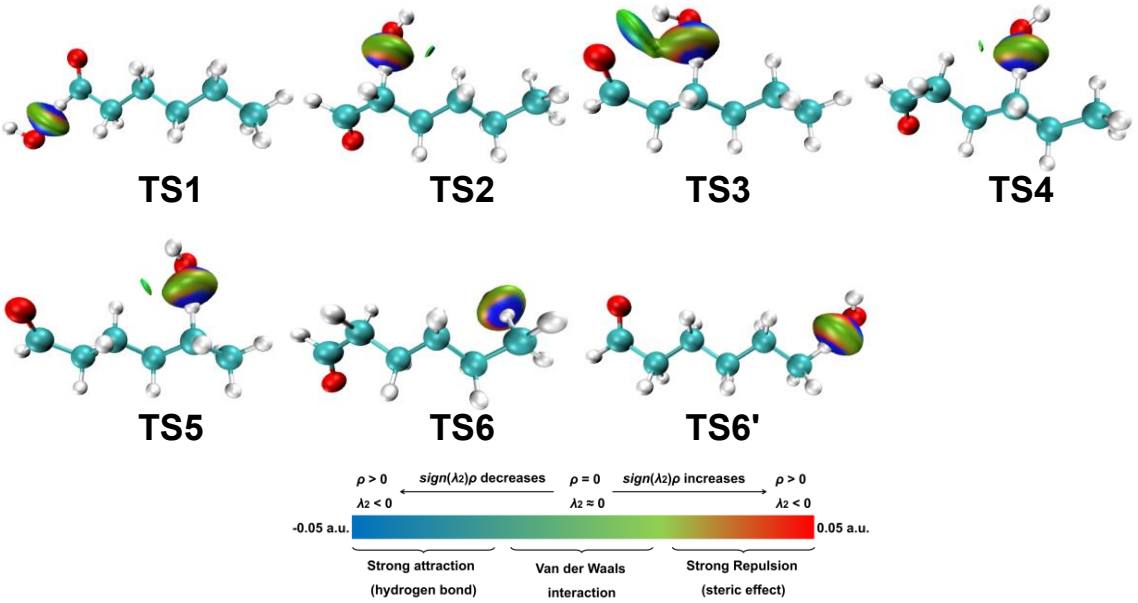

Figure S59. Intermolecular interaction of transition states in the reactions of $CH_3CH_2CH_2CH_2CH_2CHO$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

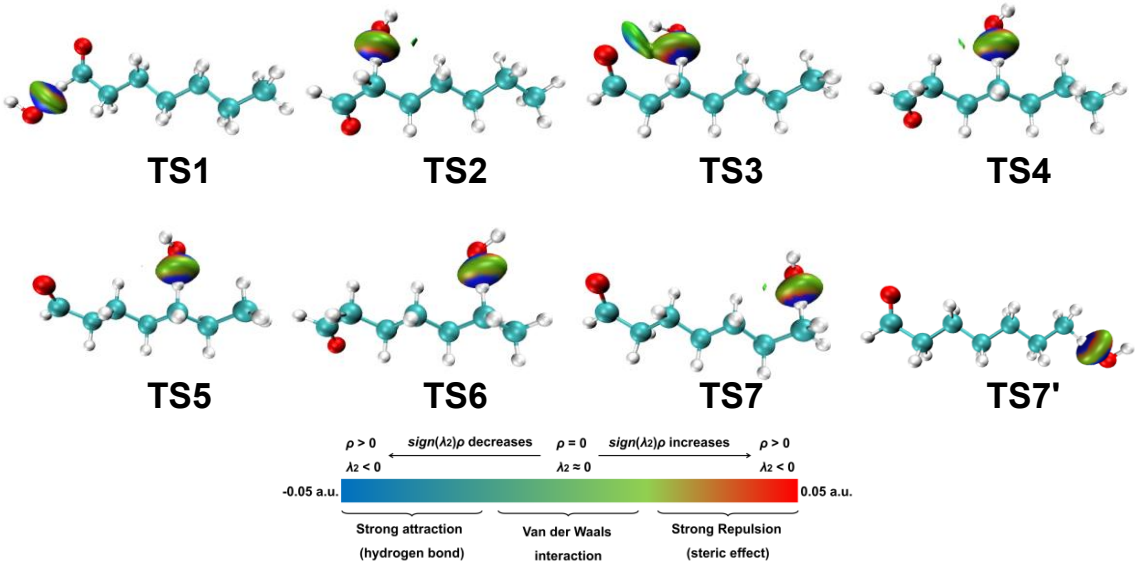

Figure S60. Intermolecular interaction of transition states in the reactions of $CH_3CH_2CH_2CH_2CH_2CH_2CHO$ with HȮ. Blue indicates hydrogen bond; green denotes the vdW interaction; red represents the spatial potential resistance.

S3 Potential energy surface of the H-abstraction reaction system

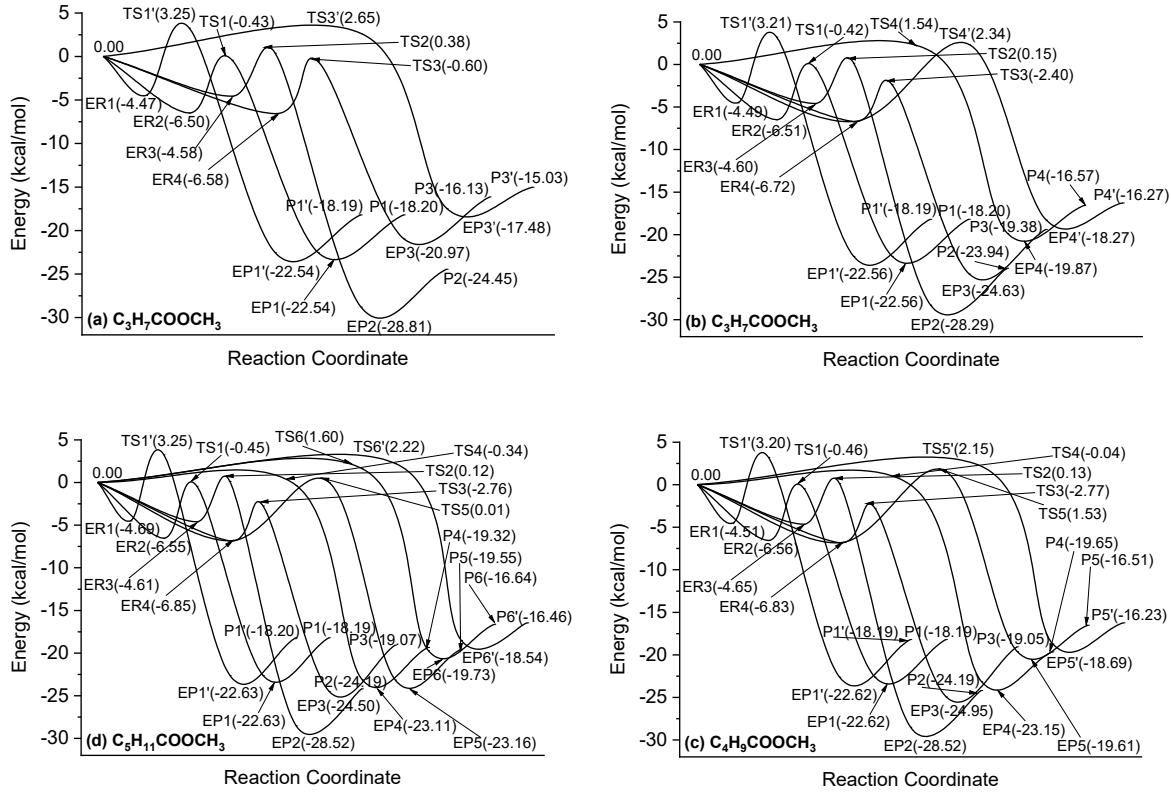

Figure S61. PES of the H-abstraction reactions of $C_nH_{2n+1}COOCH_3$ (n = 2−5) with HȮ calculated at the M06-2X/6-311++G (d, p) level.

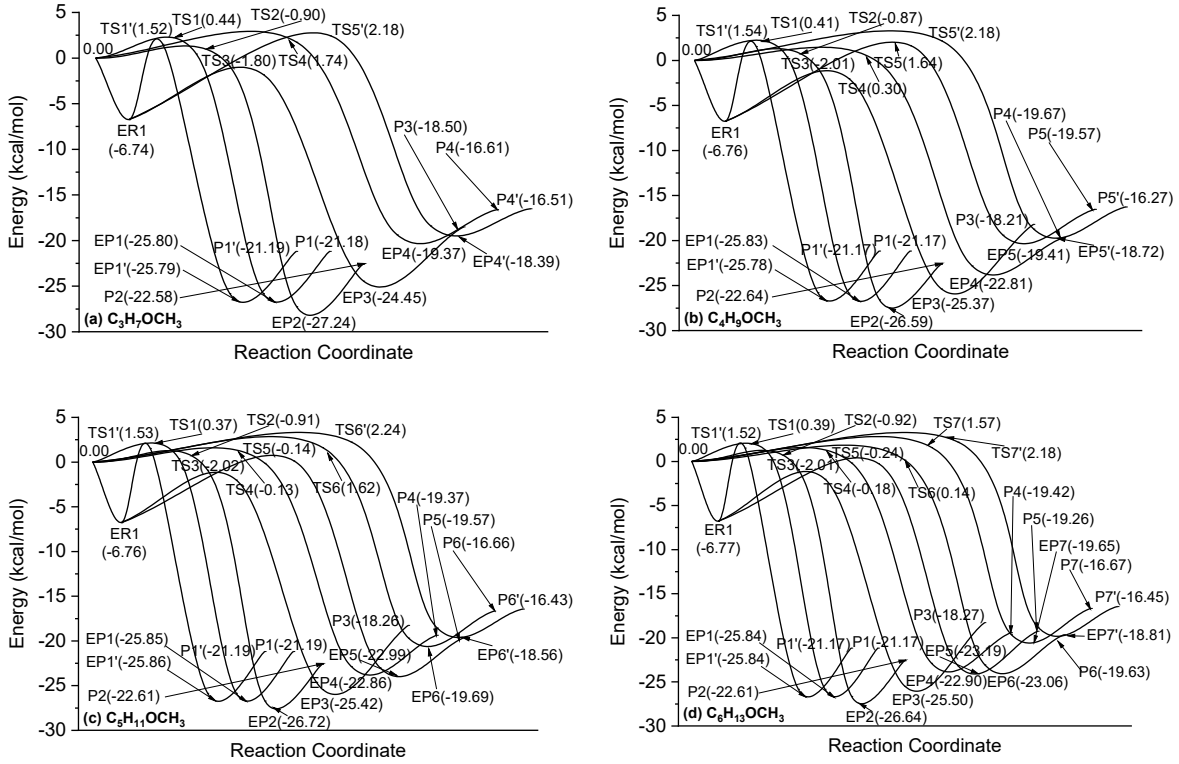

Figure S62. PES of the H-abstraction reactions of $C_nH_{2n+1}OCH_3$ (n = 3−6) with HȮ calculated at the M06-2X/6-311++G (d, p) level.

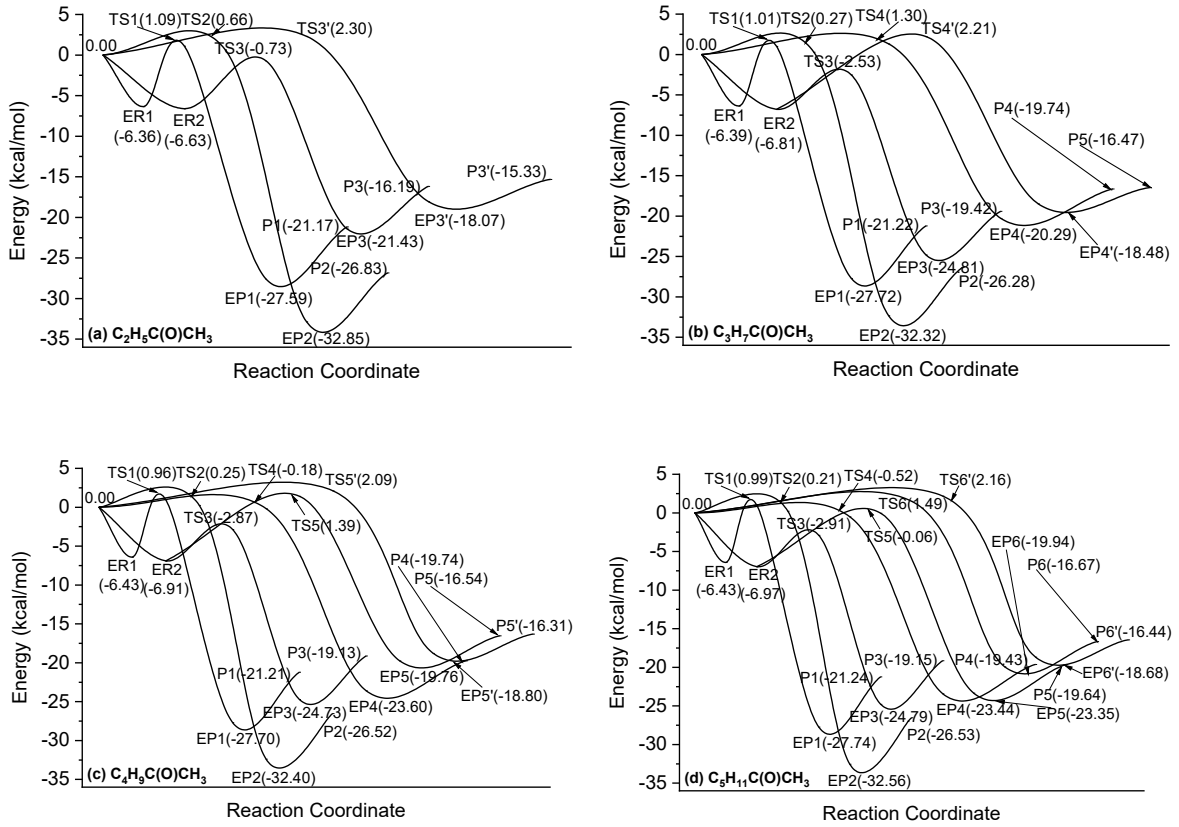

Figure S63. PES of the H-abstraction reactions of $C_nH_{2n+1}C(O)CH_3$ (n = 2−5) with HȮ calculated at the M06-2X/6-311++G (d, p) level.

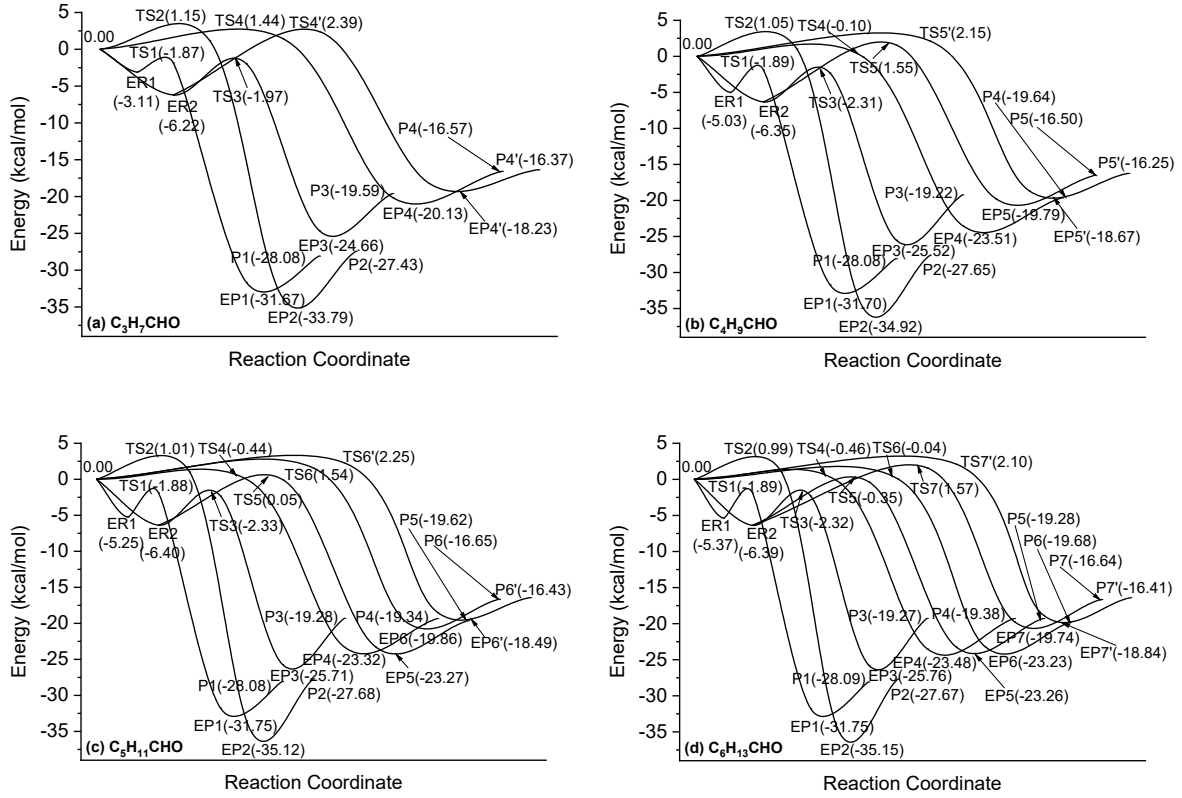

Figure S64. The PES of the H-abstraction reactions of $C_nH_{2n+1}CHO$ (n = 3−6) with HȮ calculated at the M06-2X/6-311++G (d, p) level.

S4 Individual reaction rates for H-abstraction reactions

To explore the competition among the H-abstraction reaction paths, the individual reaction rates for each H-abstraction reaction are compared in Figures S65−S68 in the Supporting Information. The reaction rates for the H-abstraction reactions in $CH_3COOC_nH_{2n+1}$ (n = 2−5) are categorized into eight types, i.e., $k_{R1'}$, k_{R1}, k_{R2}, k_{R3}, k_{RS}, k_{RE2}, k_{RE1}, and $k_{RE1'}$. The reaction rates for the H-abstraction reactions in $C_nH_{2n+1}OCH_3$ (n = 3−6) fall into eight types, i.e., $k_{R1'}$, k_{R1}, k_{R2}, k_{R3}, k_{RS}, k_{RE2}, k_{RE1}, and $k_{RE1'}$. The reaction rates for the H-abstraction reactions in $C_nH_{2n+1}C(O)CH_3$ (n = 2−5) fall into seven types, i.e., k_{R1}, k_{R2}, k_{R3}, k_{RS}, k_{RE2}, k_{RE1}, and $k_{RE1'}$. And the reaction rates for the H-abstraction reactions in $C_nH_{2n+1}CHO$ (n = 4−6) fall into eight types, i.e., k_{R1}, k_{R2}, k_{R3}, k_{RS}, k_{RE2}, k_{RE1}, and $k_{RE1'}$.

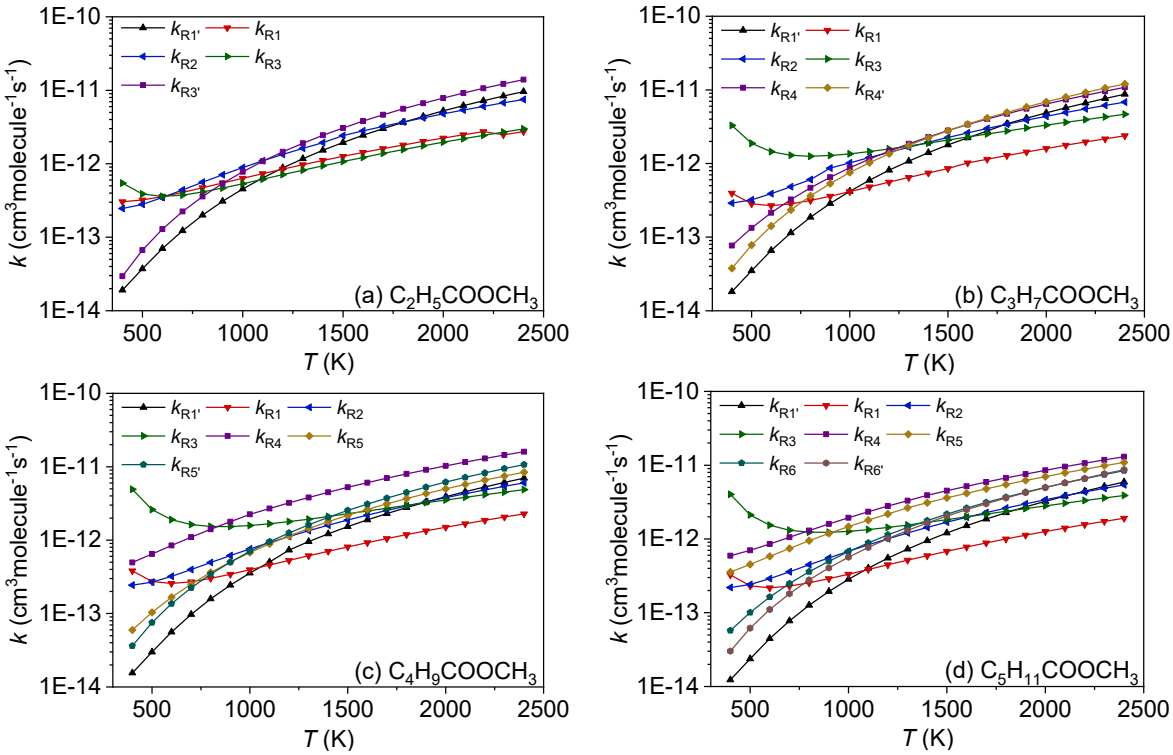

Figure S65. Individual reaction rates of $C_nH_{2n+1}COOCH_3$ (n= 2−5) over T= 400–2400 K for (a) $C_2H_5COOCH_3$, (b) $C_3H_7COOCH_3$, (c) $C_4H_9COOCH_3$, and (d) $C_5H_{11}COOCH_3$.

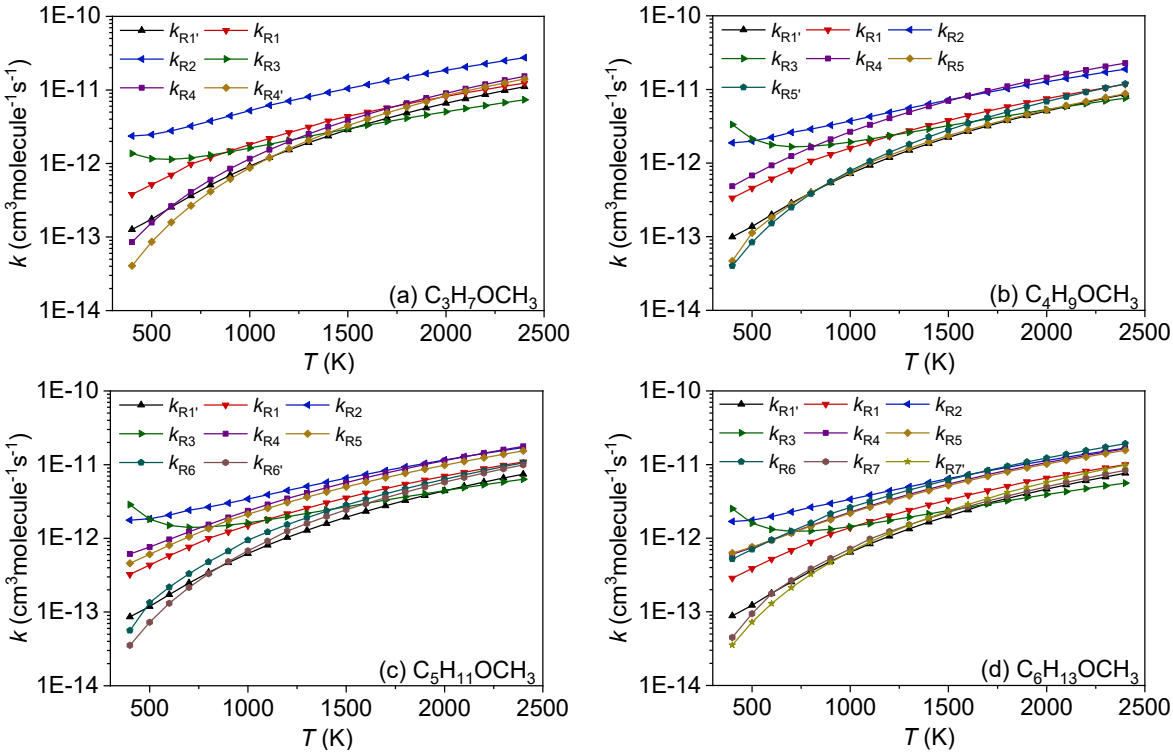

Figure S66. Individual reaction rates of $C_nH_{2n+1}OCH_3$ (n = 3−6) over T= 400–2400 K for (a) $C_3H_7OCH_3$, (b) $C_4H_9OCH_3$, (c) $C_5H_{11}OCH_3$, and (d) $C_6H_{13}OCH_3$.

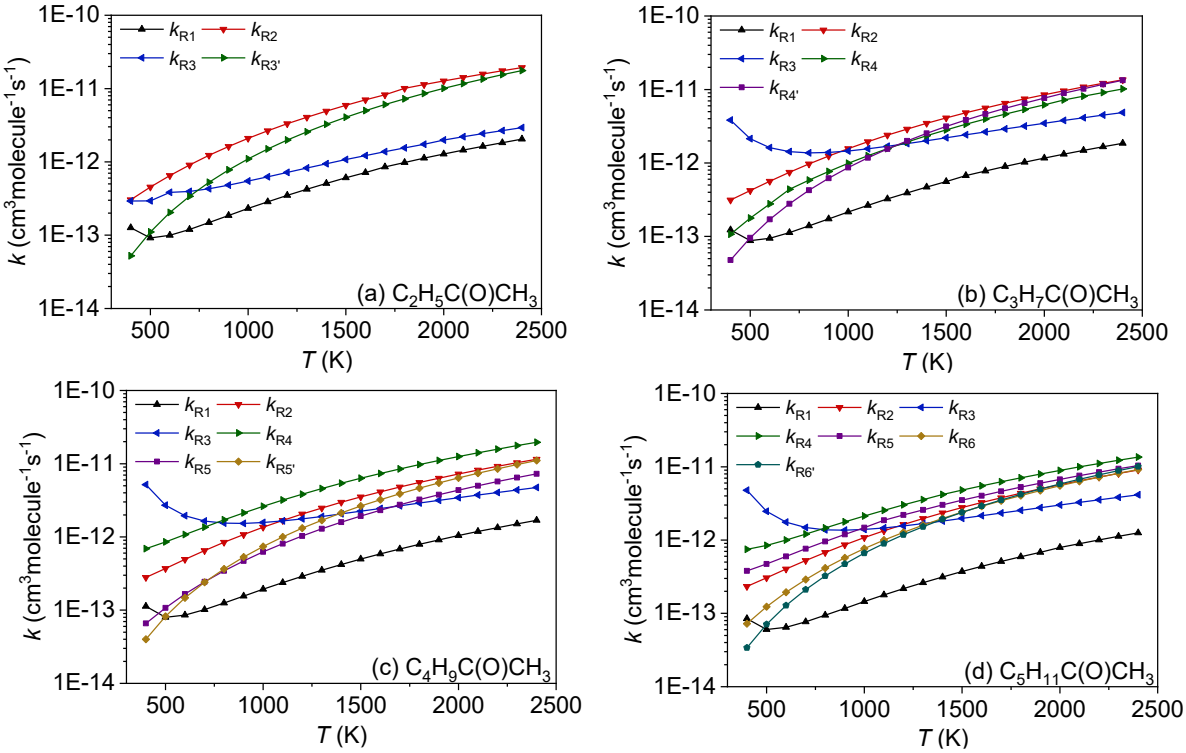

Figure S67. Individual reaction rates of $C_nH_{2n+1}C(O)CH_3$ (n = 2−5) over T= 400–2400 K for (a) $C_2H_5C(O)CH_3$, (b) $C_3H_7C(O)CH_3$, (c) $C_4H_9C(O)CH_3$, and (d) $C_5H_{11}C(O)CH_3$.

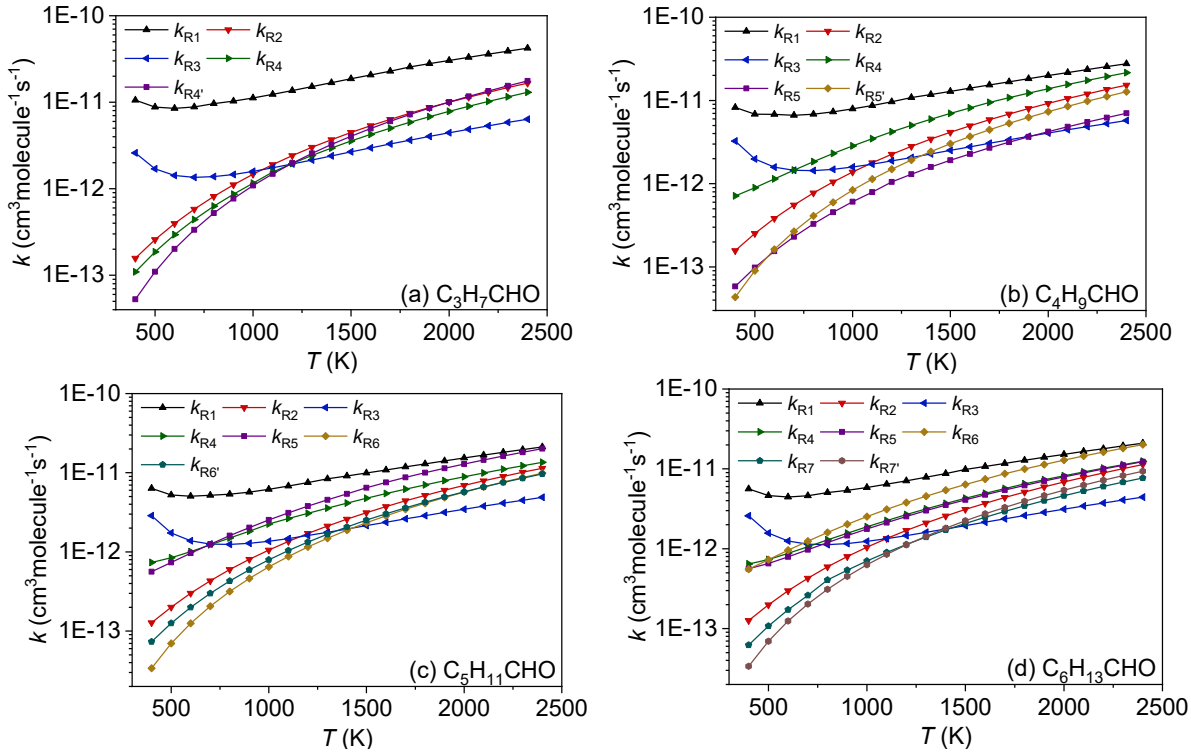

Figure S68. Individual reaction rates of $C_nH_{2n+1}CHO$ (n = 3−6) over T= 400–2400 K for (a) C_3H_7CHO, (b) C_4H_9CHO, (c) $C_5H_{11}CHO$, and (d) $C_6H_{13}CHO$.

To quantitatively assess the consistency within each characteristic pathway type, Figure S69 is constructed, in which the average rate constants for each pathway type (solid lines) are presented along with their corresponding standard deviations (error bars). The average values are calculated from all individual reaction paths belonging to each type across different chain lengths. As shown in Figure S69, the relatively small error bars for each pathway type are observed, by which the high consistency of rate constants within each category is visually confirmed. Furthermore, based on the underlying raw data, the maximum relative deviation of each individual reaction path from its corresponding characteristic pathway average is computed. The results demonstrate that this maximum deviation is consistently found to be below 35% over the entire temperature range (400−2400 K). This 35% threshold is regarded as the upper bound of the intrinsic uncertainty within each pathway type and is widely recognized as a reasonable accuracy level in kinetic rate constant calculations[1], by which its reliability as a benchmark for the classification scheme is supported. Consequently, the deviation between the rate constants predicted by our generalized rate rules and the explicitly calculated values is confirmed to be no more than 35%, by which the robustness and accuracy of the proposed classification are validated. Accordingly, this 35% threshold is also adopted as the criterion for identifying functional group effects in the comparative analysis between oxygenated

fuels and alkanes. Reaction pathways with relative deviations from the corresponding alkane rate constants within ±35% are classified as alkane-like (i.e., are considered unaffected by the functional group), while those exceeding this threshold are identified as functionally influenced.

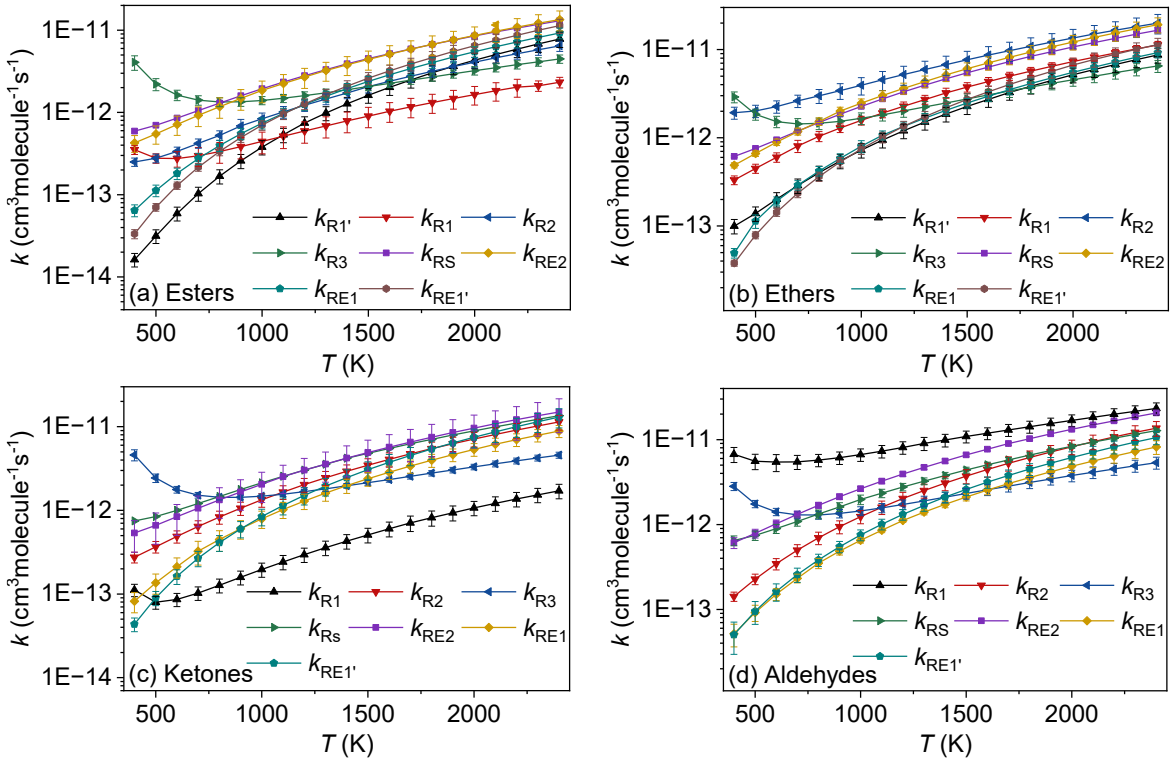

Figure S69. Characteristic reaction rates over T= 400–2400 K for (a) esters, (b) ethers, (c) ketones, and (d) aldehydes. The solid lines represent the average rate constants calculated from all individual reaction paths belonging to each type across different chain lengths (C4−C7), and the error bars denote the corresponding standard deviations.

S5 Computational workflow

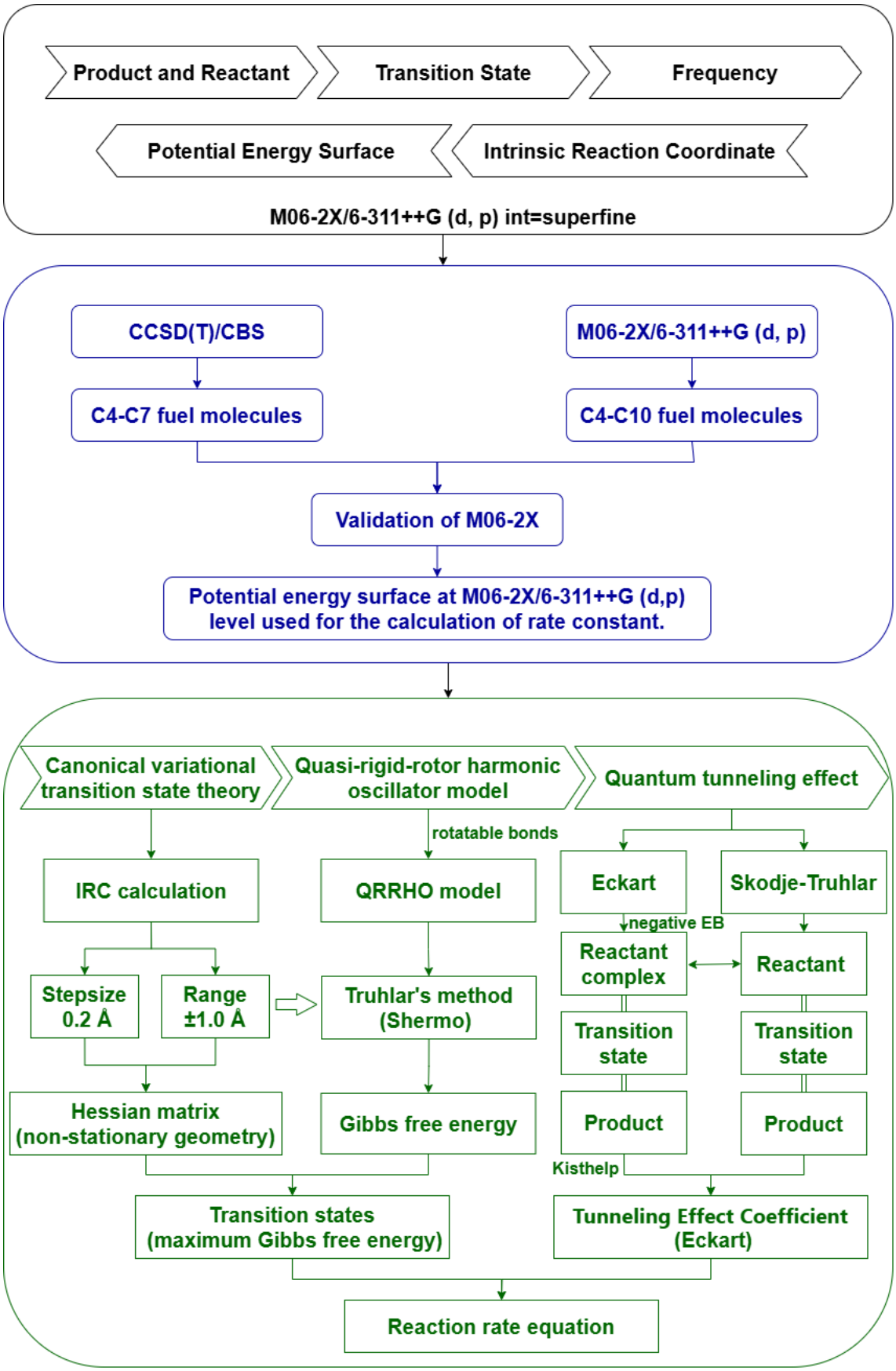

Table S3. Summary of computational methods applied to alkanes and oxygenated fuels

Computational aspect	Alkanes	Oxygenated fuels
Geometry optimization	M06-2X/6-311++G (d, p)	M06-2X/6-311++G (d, p)
Frequency calculation	M06-2X/6-311++G (d, p)	M06-2X/6-311++G (d, p)
Frequency scaling factor	0.983	0.983
IRC analysis	M06-2X/6-311++G (d, p)	M06-2X/6-311++G (d, p)
Low-frequency mode treatment	Quasi-RRHO (Shermo)	Quasi-RRHO (Shermo)
High-level benchmark	-	CCSD(T)/CBS (C4–C5)
PES for kinetics	M06-2X/6-311++G (d, p)	M06-2X/6-311++G (d, p)
Rate constant theory	CVT + Eckart	CVT + Eckart
Temperature range	400−2400 K	400−2400 K

S6 Vibrational frequencies of transition state structures

1. Esters

All frequencies are in cm^{-1}.

(1) $C_2H_5C(O)OCH_3$

TS1'

-1264.4	21.0	53.9	78.1	133.3	164.5	189.1	220.4	303.6
321.0	444.8	577.5	644.3	733.3	814.4	882.7	924.2	1021.8
1067.9	1114.9	1131.9	1151.8	1229.2	1254.8	1280.3	1285.1	1397.8
1425.6	1467.0	1485.5	1498.7	1506.8	1531.2	1865.2	3081.2	3083.3
3106.4	3116.1	3160.1	3161.8	3194.7	3805.3			

TS1

-1211.0	47.7	63.3	139.1	182.7	213.5	228.7	340.1	346.3
405.9	455.6	584.1	666.1	795.3	816.2	897.4	902.0	1016.6
1079.1	1116.3	1137.7	1141.7	1240.8	1256.0	1285.5	1374.2	1402.8
1427.0	1465.3	1471.9	1499.7	1504.6	1510.6	1844.4	3081.7	3083.7
3116.6	3117.2	3160.7	3161.6	3216.4	3765.7			

TS2

-992.6	50.1	105.0	133.2	149.7	168.8	210.1	224.1	320.6
338.9	438.8	594.7	643.8	668.5	846.1	875.9	934.5	1030.1
1074.7	1097.2	1148.3	1187.7	1218.7	1246.4	1303.2	1363.4	1415.8
1480.1	1487.6	1491.9	1495.3	1510.5	1526.5	1859.0	3074.1	3089.1
3118.4	3145.8	3167.3	3167.6	3200.5	3782.4			

TS3

-1172.0	39.4	108.0	148.4	162.3	180.1	215.5	344.0	359.1
440.8	460.5	584.7	661.1	763.2	850.4	920.2	945.8	1020.6
1066.1	1102.1	1143.3	1188.3	1219.4	1252.7	1274.3	1322.2	1410.9
1447.4	1454.9	1466.7	1489.8	1497.6	1509.4	1833.6	3074.7	3089.7
3108.8	3118.3	3167.3	3189.5	3203.9	3754.8			

TS3'

-838.5	37.2	52.1	60.8	100.5	152.5	177.1	194.5	308.4
347.1	444.2	586.1	663.8	751.2	820.4	906.8	982.4	1036.6
1098.4	1115.7	1187.8	1205.1	1219.4	1252.8	1280.1	1316.2	1390.4
1410.4	1467.0	1479.7	1487.1	1496.7	1510.0	1849.7	3086.8	3089.2
3117.6	3127.6	3163.2	3187.7	3200.2	3807.0			

(2) $C_3H_7C(O)OCH_3$

TS1'

-1265.7	18.3	47.0	68.6	80.6	131.6	146.8	176.4	242.4
266.2	320.1	343.5	433.0	581.3	663.7	751.7	768.0	884.8
889.0	922.0	964.3	1070.4	1076.7	1130.3	1150.4	1152.3	1218.5
1253.8	1254.9	1280.7	1329.1	1338.6	1417.0	1423.9	1464.0	1485.5

1496.0 1506.0 1512.6 1531.6 1864.1 3060.2 3067.8 3085.3 3099.7
3106.1 3116.8 3137.7 3142.7 3194.3 3805.2

TS1

-1207.5 42.2 50.0 99.7 125.0 165.7 201.7 247.1 312.3
345.8 350.0 407.0 445.9 588.4 704.2 753.1 811.7 889.0
900.1 920.4 942.3 1070.7 1090.1 1131.7 1142.3 1153.3 1234.9
1249.2 1255.7 1328.7 1341.8 1376.5 1418.2 1425.9 1462.2 1471.8
1496.5 1507.0 1508.4 1513.3 1843.1 3060.7 3068.4 3084.8 3100.0
3117.1 3117.2 3137.7 3143.3 3216.2 3766.8

TS2

-936.5 44.6 74.0 100.0 112.5 142.4 161.5 189.7 250.1
310.6 321.1 343.4 428.5 597.8 655.1 718.0 772.8 895.1
899.1 948.4 971.1 1060.2 1084.3 1123.3 1167.2 1187.9 1217.3
1238.4 1271.9 1314.6 1327.1 1395.4 1420.4 1479.2 1483.7 1495.9
1504.2 1508.0 1510.2 1511.9 1857.9 3063.0 3067.1 3089.0 3099.5
3114.1 3136.9 3146.5 3167.1 3200.3 3781.1

TS3

-832.7 34.9 81.8 125.6 151.6 154.4 168.0 191.6 231.7
318.6 346.8 432.7 454.9 594.5 681.1 726.7 767.0 906.3
934.2 944.7 1056.0 1062.9 1095.7 1139.9 1149.5 1187.8 1218.7
1256.1 1258.1 1313.3 1353.9 1410.7 1414.1 1447.1 1454.8 1489.2
1495.5 1497.0 1502.1 1509.5 1832.3 3053.1 3064.5 3089.4 3099.9
3111.8 3124.3 3151.7 3166.9 3203.2 3750.3

TS4

-748.3 30.7 53.3 81.6 104.4 123.7 150.7 157.4 184.8
320.9 324.7 350.5 443.9 593.6 691.6 719.5 786.2 888.6
916.1 939.0 1052.7 1068.8 1103.3 1141.1 1187.7 1200.4 1220.6
1248.1 1301.3 1322.6 1334.0 1360.8 1424.2 1441.3 1469.3 1485.0
1488.0 1491.2 1496.4 1510.5 1851.3 3065.3 3074.3 3085.8 3092.5
3107.9 3126.3 3161.1 3164.7 3198.0 3804.9

TS4'

-866.4 26.4 36.3 64.9 79.8 89.4 154.0 156.3 183.7
296.4 336.2 352.5 442.5 592.3 690.7 726.1 757.3 888.3
921.6 956.2 1035.4 1073.9 1092.1 1127.1 1187.9 1216.2 1238.5
1242.8 1278.0 1318.6 1329.9 1356.6 1416.0 1426.0 1465.1 1476.9
1487.1 1496.7 1503.0 1510.4 1853.1 3071.6 3080.1 3087.1 3092.0
3105.7 3126.0 3162.2 3163.2 3200.0 3804.2

(3) $C_4H_9C(O)OCH_3$

TS1'

-1261.7 17.1 40.4 61.5 69.3 113.6 119.9 131.3 174.2
233.4 243.9 312.4 320.3 329.8 493.2 579.9 662.8 733.9
764.3 808.6 887.7 916.4 941.6 964.6 1043.9 1081.6 1093.9
1137.3 1149.3 1152.6 1215.1 1237.8 1254.4 1281.0 1301.1 1316.4
1332.9 1383.7 1417.5 1426.5 1463.9 1485.5 1491.6 1500.1 1504.7

1513.9 1531.4 1864.0 3048.3 3061.0 3066.4 3075.2 3078.7 3099.7
3106.1 3120.2 3132.4 3139.3 3194.1 3805.1

TS1

-1206.4 31.2 47.9 89.6 97.6 121.4 151.5 199.4 247.5
262.2 315.7 346.4 357.0 405.7 498.2 587.3 701.3 735.2
807.9 812.4 898.0 911.7 941.8 946.5 1046.0 1089.3 1098.1
1138.4 1142.7 1152.1 1231.7 1238.3 1247.7 1305.8 1316.5 1333.1
1374.0 1387.8 1417.6 1428.9 1462.0 1471.9 1491.9 1500.3 1505.2
1508.8 1514.4 1843.0 3048.9 3061.0 3066.6 3075.1 3079.3 3100.0
3117.0 3120.0 3132.4 3139.6 3216.0 3766.5

TS2

-934.7 40.7 66.6 72.1 94.1 111.4 148.0 163.3 187.3
247.2 270.6 309.6 314.7 358.2 465.1 601.4 663.4 717.1
745.6 830.4 905.5 927.6 939.5 966.0 1038.6 1076.5 1102.4
1137.4 1166.1 1188.0 1215.6 1233.4 1253.1 1294.7 1314.4 1330.3
1367.3 1409.5 1417.9 1478.5 1480.9 1496.2 1497.6 1505.3 1506.5
1511.0 1512.8 1857.8 3050.0 3057.1 3061.4 3084.6 3089.0 3099.9
3112.6 3131.7 3140.2 3167.0 3200.2 3781.1

TS3

-794.9 31.0 58.7 94.6 107.4 137.4 148.0 160.6 187.2
250.5 267.3 313.6 369.0 437.6 490.7 598.8 693.2 721.1
753.6 809.8 914.3 942.3 972.8 1036.3 1071.0 1093.3 1109.5
1140.8 1165.9 1188.0 1218.3 1238.8 1252.5 1293.0 1316.7 1334.8
1384.9 1403.6 1418.4 1436.0 1454.4 1485.5 1489.1 1497.2 1504.9
1509.3 1510.3 1831.8 3036.9 3063.8 3064.7 3079.0 3089.3 3096.7
3110.2 3135.9 3145.1 3166.8 3203.1 3747.5

TS4

-530.2 26.8 47.5 71.3 90.5 107.9 114.3 130.0 156.2
181.9 236.5 267.7 314.7 360.6 496.4 593.3 627.6 716.1
775.7 831.7 902.9 935.3 945.5 1039.6 1071.7 1089.7 1128.9
1149.1 1187.9 1196.7 1215.0 1232.5 1239.5 1303.9 1320.8 1366.6
1385.3 1412.7 1426.4 1469.7 1484.6 1489.0 1496.4 1496.6 1500.5
1510.8 1641.4 1851.2 3055.8 3059.6 3073.4 3075.1 3085.6 3102.6
3120.4 3125.3 3145.8 3160.7 3197.5 3800.7

TS5

-785.5 24.8 45.2 74.1 90.0 116.0 143.3 156.4 171.3
185.9 267.2 314.5 329.2 362.9 498.2 590.9 714.4 729.9
793.3 811.7 895.2 926.6 946.8 1038.8 1064.5 1093.7 1112.4
1142.0 1180.4 1188.1 1216.5 1232.5 1244.1 1298.1 1313.8 1330.4
1350.6 1389.0 1425.5 1450.1 1465.7 1478.1 1485.7 1486.9 1496.6
1506.3 1510.6 1852.1 3036.0 3066.6 3074.2 3083.4 3086.3 3095.2
3103.5 3124.3 3161.8 3162.4 3198.7 3799.7

TS5'

-723.3 29.9 35.2 42.6 70.9 98.8 113.8 121.1 156.0
183.0 256.6 301.9 334.3 361.0 492.0 589.6 703.2 722.3

738.7 811.9 923.5 935.2 983.3 1038.6 1061.6 1078.1 1113.3
1137.3 1187.8 1214.2 1224.1 1239.2 1244.9 1294.0 1313.7 1329.4
1335.5 1381.8 1422.2 1437.4 1465.2 1483.4 1487.5 1496.0 1496.5
1507.7 1510.6 1852.8 3058.9 3069.3 3078.0 3086.3 3090.6 3091.9
3104.9 3125.1 3158.2 3161.8 3198.5 3806.8

(4) $C_5H_{11}C(O)OCH_3$

TS1'

-1261.7 10.8 38.2 50.2 54.5 97.1 108.3 126.2 155.4
182.3 194.3 247.1 265.1 302.7 320.9 411.9 500.6 580.6
663.4 729.6 764.7 766.3 857.5 888.1 912.9 965.4 977.2
1033.8 1067.9 1089.2 1097.1 1141.0 1151.8 1152.1 1212.9 1227.3
1254.8 1277.8 1280.8 1294.1 1331.5 1336.6 1350.3 1405.1 1416.0
1427.1 1463.8 1485.4 1489.0 1493.2 1504.6 1505.4 1514.2 1530.5
1863.9 3034.2 3053.8 3059.2 3064.7 3066.7 3075.6 3090.6 3100.7

TS1

-1205.6 30.0 37.2 71.2 77.7 110.0 135.1 143.2 201.1
211.9 246.1 275.9 335.1 346.2 402.4 419.2 505.3 587.2
702.3 730.9 765.9 811.1 857.8 898.2 908.9 945.0 977.6
1036.2 1071.9 1089.7 1105.2 1140.3 1144.1 1153.6 1227.6 1228.8
1246.7 1283.1 1294.0 1331.5 1337.0 1351.8 1376.2 1406.6 1415.9
1428.9 1462.0 1471.9 1489.5 1493.6 1504.7 1505.0 1509.1 1514.6
1842.9 3034.8 3053.7 3059.2 3065.2 3066.9 3075.5 3090.6 3101.0
3116.9 3121.4 3129.0 3137.4 3216.0 3766.7

TS2

-933.8 36.8 47.1 63.7 78.8 104.5 124.3 146.4 160.9
183.7 213.7 247.9 276.8 304.6 337.3 410.6 478.1 601.3
663.8 717.1 734.5 782.9 868.6 899.6 938.8 959.6 973.0
1032.3 1058.2 1090.9 1104.1 1142.3 1168.5 1187.8 1214.5 1230.1
1239.2 1277.7 1302.1 1321.8 1335.8 1340.6 1388.7 1416.1 1417.3
1478.4 1480.5 1491.5 1496.1 1500.9 1505.3 1507.2 1511.2 1513.7
1857.7 3038.9 3051.8 3056.0 3059.6 3071.4 3088.9 3090.2 3100.8
3113.4 3129.6 3137.3 3167.0 3200.1 3780.9

TS3

-795.9 31.4 49.3 67.7 79.9 115.6 144.5 155.6 162.4
189.4 216.6 246.3 280.7 344.8 409.2 446.4 496.3 598.2
698.4 721.7 749.0 770.7 868.7 906.3 941.8 988.0 1028.5
1066.3 1086.2 1100.9 1106.7 1146.9 1166.6 1187.9 1218.1 1228.9
1248.6 1273.0 1297.0 1324.5 1337.4 1359.9 1402.4 1405.5 1416.4
1435.3 1454.4 1481.7 1489.3 1497.0 1498.0 1505.7 1509.6 1512.2
1831.7 3023.1 3056.1 3058.9 3064.7 3067.9 3089.4 3094.2 3100.1

TS4

-496.4 26.4 44.1 56.6 71.6 84.4 113.0 121.9 137.6
158.2 185.8 206.7 253.3 276.3 341.3 418.6 504.0 593.0
624.9 716.9 762.5 780.2 879.9 906.5 941.1 973.4 1031.7

1060.6 1092.9 1096.1 1134.7 1151.1 1187.7 1204.2 1215.2 1227.5
1237.8 1285.9 1297.1 1328.2 1340.7 1368.7 1399.4 1413.0 1426.2
1469.1 1482.3 1486.8 1492.9 1495.9 1504.7 1509.8 1510.8 1651.2
1851.3 3045.0 3058.1 3059.9 3060.7 3073.3 3085.6 3091.3 3102.7
3120.7 3128.8 3140.3 3160.8 3197.5 3798.1

TS5

-540.5 23.2 39.4 63.8 74.3 93.8 120.9 128.5 152.0
159.7 185.4 208.4 238.6 276.6 341.2 412.2 505.8 590.7
636.8 715.4 740.9 804.1 874.0 910.4 941.6 973.2 1031.1
1067.9 1089.6 1096.5 1136.4 1149.6 1188.0 1214.3 1219.1 1235.5
1242.8 1282.1 1303.1 1323.2 1340.1 1348.3 1399.9 1411.3 1426.2
1465.9 1481.3 1486.9 1495.1 1496.7 1499.8 1505.6 1510.8 1582.1
1851.9 3028.2 3054.7 3066.2 3068.7 3075.1 3085.7 3086.2 3102.4
3122.8 3123.8 3147.6 3161.7 3198.5 3794.9

TS6

-740.0 23.5 36.7 56.0 81.7 84.4 89.7 124.3 151.3
161.0 184.5 211.6 277.1 321.6 340.7 417.8 505.9 589.6
715.1 720.2 748.9 796.7 864.6 895.9 934.1 978.9 1027.1
1060.8 1085.3 1093.3 1124.4 1143.1 1185.6 1187.9 1215.1 1232.4
1241.8 1280.6 1291.0 1323.9 1332.1 1347.2 1359.4 1406.2 1427.2
1457.0 1465.0 1481.7 1486.4 1493.3 1496.4 1502.0 1510.1 1511.1
1853.5 3034.0 3039.8 3066.6 3073.4 3077.1 3085.8 3087.2 3096.6
3102.8 3122.1 3159.2 3161.1 3197.8 3804.9

TS6'

-799.7 22.9 43.6 48.5 57.9 73.7 100.6 127.4 131.1
157.2 184.7 195.4 273.3 333.4 346.5 400.8 500.5 590.3
707.8 727.1 734.1 771.7 859.2 919.4 942.2 978.7 1020.0
1061.1 1064.1 1086.9 1117.1 1140.2 1188.1 1213.3 1219.5 1231.7
1266.6 1284.4 1310.7 1331.8 1332.4 1336.2 1367.5 1399.7 1425.9
1437.1 1465.5 1477.1 1486.5 1491.8 1496.7 1497.1 1510.4 1511.1
1853.4 3039.3 3053.3 3067.8 3071.7 3076.5 3086.2 3089.0 3096.2
3103.5 3123.2 3157.9 3161.8 3198.6 3805.6

(5) $C_6H_{13}C(O)OH$

TS1

-1774.1 18.8 39.4 61.4 71.9 98.7 139.0 148.9 150.5
224.9 246.3 250.2 338.1 398.4 425.4 457.8 494.7 582.5
637.4 729.7 745.2 757.6 806.5 896.2 907.8 918.5 946.0
1001.4 1035.6 1060.7 1081.9 1092.0 1137.8 1141.3 1179.3 1220.1
1252.4 1276.1 1308.1 1318.8 1333.4 1338.6 1362.2 1399.3 1413.6
1416.9 1462.9 1488.6 1489.4 1497.6 1504.9 1507.4 1514.8 1583.4
1790.3 3035.4 3041.4 3052.7 3059.3 3063.4 3073.5 3077.0 3082.9
3095.6 3110.6 3129.1 3130.8 3136.8 3723.9

TS2

-957.2 39.9 47.6 54.6 68.6 105.8 122.5 127.3 167.9

189.6 247.5 256.6 291.8 354.3 453.0 486.9 533.0 640.6
649.6 672.3 731.4 753.7 818.3 885.4 903.5 923.2 955.9
997.3 1040.1 1066.7 1090.3 1099.0 1142.3 1155.6 1185.6 1227.5
1251.2 1284.8 1293.6 1311.8 1333.6 1335.2 1341.5 1376.6 1403.3
1415.3 1419.9 1478.4 1489.5 1494.0 1498.6 1505.0 1505.4 1514.6
1878.7 3035.7 3042.4 3052.6 3055.2 3058.9 3065.0 3079.8 3094.1
3102.2 3114.7 3128.7 3136.4 3780.8 3829.8

TS3

-788.0 38.9 44.2 60.2 70.5 102.5 141.4 150.2 158.4
201.1 247.2 258.4 348.3 429.8 452.1 498.2 537.0 651.5
666.0 696.9 736.5 762.6 805.6 901.8 911.7 919.3 1005.7
1041.1 1061.7 1088.0 1096.2 1107.9 1146.1 1166.7 1199.0 1222.6
1254.9 1273.7 1299.7 1309.3 1330.9 1337.5 1348.1 1389.1 1413.8
1415.9 1418.0 1446.3 1454.6 1481.6 1491.9 1501.7 1504.7 1513.9
1855.2 3024.3 3041.8 3051.2 3059.5 3064.9 3066.8 3076.5 3095.2
3100.1 3110.2 3129.9 3136.7 3755.2 3825.8

TS4

-504.5 30.2 48.2 54.3 60.7 73.4 90.9 130.7 135.3
166.2 193.0 246.7 256.8 351.1 456.6 510.4 520.4 625.5
648.0 653.1 740.2 777.7 818.2 900.2 908.7 918.8 995.4
1038.4 1070.7 1086.7 1094.6 1136.0 1144.0 1182.9 1201.3 1223.5
1260.9 1280.3 1295.2 1319.0 1334.2 1340.4 1363.8 1387.2 1409.7
1416.2 1440.3 1467.1 1480.0 1491.2 1497.9 1505.4 1511.7 1643.0
1872.1 3031.2 3048.7 3060.1 3060.8 3061.2 3072.9 3074.4 3093.6
3102.6 3120.6 3130.5 3138.2 3797.7 3832.6

TS5

-523.6 25.6 42.6 57.9 75.0 79.4 83.0 124.4 132.3
159.7 193.9 249.5 257.2 353.5 456.8 513.4 523.2 632.2
650.5 653.7 739.9 776.6 813.4 898.9 908.7 928.1 1001.4
1041.7 1062.0 1089.6 1099.2 1138.1 1144.9 1184.1 1212.5 1233.2
1257.9 1286.6 1299.3 1315.1 1333.5 1335.1 1360.5 1387.6 1408.8
1416.3 1439.3 1464.5 1479.4 1488.7 1504.0 1506.2 1510.9 1589.2
1873.3 3029.8 3041.3 3060.6 3061.8 3066.6 3073.7 3078.4 3090.3
3101.9 3123.4 3132.5 3142.3 3794.9 3831.7

TS6

-677.7 26.4 37.9 63.3 75.3 80.9 97.4 116.9 138.9
152.1 195.2 235.4 257.0 353.5 456.7 512.1 519.9 617.8
649.2 651.0 733.6 764.3 816.4 899.3 902.8 921.9 992.5
1039.7 1067.6 1092.6 1096.9 1132.5 1144.5 1180.4 1194.0 1244.4
1257.3 1279.7 1296.1 1329.7 1336.5 1340.1 1381.7 1406.0 1413.4
1418.7 1439.9 1463.6 1482.1 1492.8 1498.7 1501.2 1509.4 1638.7
1873.2 3029.5 3042.2 3052.8 3063.8 3066.9 3075.0 3079.9 3088.8
3101.6 3116.9 3121.6 3138.7 3801.1 3832.4

TS7

-752.2 23.9 38.9 60.6 62.6 86.1 110.3 117.4 136.2

165.1 192.0 258.6 323.5 352.5 457.5 511.8 518.9 647.3
651.1 725.6 738.9 783.9 815.5 881.8 902.9 917.0 994.6
1035.6 1062.8 1084.2 1095.3 1124.7 1143.6 1171.4 1190.4 1227.6
1258.5 1269.8 1298.5 1312.8 1332.9 1335.4 1347.4 1351.5 1391.3
1415.3 1439.5 1454.6 1463.8 1479.6 1489.6 1492.7 1498.2 1511.5
1874.1 3034.3 3035.3 3043.4 3066.3 3067.2 3075.7 3079.5 3090.2
3098.4 3102.8 3122.0 3159.5 3803.1 3831.8

TS7'

-706.6 25.4 35.8 39.8 64.5 76.3 87.5 91.0 138.0
151.6 195.3 237.0 329.4 356.8 444.8 512.4 520.6 650.3
650.8 708.5 730.2 748.6 808.9 894.6 903.9 968.9 1001.2
1033.0 1064.3 1082.3 1086.4 1112.4 1143.2 1177.8 1215.7 1229.2
1257.3 1274.9 1295.0 1316.8 1324.6 1335.5 1338.4 1348.7 1385.5
1410.5 1439.6 1443.7 1463.9 1484.4 1489.7 1497.3 1502.4 1512.6
1874.1 3037.0 3044.9 3063.0 3066.3 3067.2 3076.1 3083.4 3088.4
3100.1 3107.4 3122.4 3155.4 3807.1 3831.9

(6) $C_4H_9C(O)OC_2H_5$

TS1'

-988.2 21.6 36.5 48.6 71.2 80.9 91.9 100.8 120.1
176.7 188.6 249.7 290.5 334.7 344.6 381.2 499.0 587.1
722.1 733.4 765.7 807.9 837.3 886.5 920.6 940.9 971.5
1003.3 1054.2 1088.7 1095.8 1137.3 1143.9 1173.8 1197.4 1218.8
1237.0 1297.4 1302.5 1310.8 1315.2 1331.4 1379.9 1399.8 1412.3
1416.4 1434.4 1464.2 1484.1 1491.1 1500.2 1505.5 1514.0 1522.1
1853.6 3047.7 3060.4 3066.4 3074.9 3078.0 3091.0 3099.4 3112.9
3119.7 3131.7 3137.0 3138.4 3188.8 3805.0

TS1

-1138.2 28.0 45.7 58.6 76.5 97.0 121.3 135.3 186.2
204.2 247.0 289.6 300.5 333.0 377.6 388.9 498.5 586.1
702.1 734.0 736.5 809.8 855.2 902.8 923.0 942.1 970.8
983.1 1052.4 1085.9 1094.7 1137.7 1145.0 1160.3 1199.4 1217.3
1238.0 1285.4 1301.7 1317.0 1322.4 1332.8 1381.3 1411.1 1417.1
1432.3 1459.3 1464.4 1491.9 1500.5 1503.4 1505.1 1512.9 1514.6
1861.1 3048.2 3060.8 3064.0 3074.1 3078.8 3081.7 3098.3 3113.6
3119.7 3131.6 3132.2 3139.2 3191.6 3786.5

TS2

-889.7 28.9 47.5 79.8 90.1 115.0 128.2 158.4 172.7
203.6 245.6 265.0 298.4 334.8 386.5 411.3 500.6 587.6
646.3 728.6 735.8 809.2 866.5 909.4 935.6 942.0 954.1
976.7 1055.3 1092.7 1123.8 1138.8 1154.2 1161.0 1165.8 1237.5
1238.2 1307.2 1316.3 1316.9 1333.1 1381.2 1399.1 1417.4 1423.4
1438.1 1462.5 1485.3 1492.2 1496.2 1500.6 1504.9 1514.4 1518.9
1838.8 3048.6 3060.8 3066.5 3071.4 3075.0 3079.0 3099.9 3114.2
3119.9 3132.2 3139.2 3147.1 3165.7 3762.1

TS3

-943.3 27.5 63.7 71.5 73.0 88.0 98.4 142.7 173.2
201.4 245.2 263.5 297.1 308.3 333.4 389.6 471.6 602.0
662.2 725.6 746.4 813.2 831.7 896.0 924.2 936.0 942.2
987.8 1058.7 1083.4 1104.0 1135.4 1150.6 1166.0 1185.0 1222.9
1252.6 1293.4 1312.1 1314.6 1329.9 1365.3 1400.9 1409.8 1417.7
1437.9 1479.9 1493.0 1497.6 1503.7 1504.6 1506.1 1512.7 1529.6
1853.9 3050.0 3057.1 3061.3 3075.1 3084.2 3092.1 3099.1 3111.8
3131.6 3132.3 3139.9 3153.9 3160.0 3777.7

TS4

-795.0 25.3 58.3 80.7 90.2 95.9 130.8 145.8 159.7
207.6 248.8 265.7 294.2 339.2 401.0 441.4 494.3 597.3
694.6 731.1 755.2 808.9 817.1 899.8 932.7 970.2 977.6
1050.6 1082.4 1095.2 1109.7 1138.0 1152.8 1167.1 1185.3 1238.5
1245.4 1292.7 1313.3 1316.3 1334.6 1380.7 1397.9 1409.3 1418.6
1432.1 1447.8 1456.6 1486.3 1491.9 1504.5 1504.7 1510.5 1528.9
1827.3 3036.8 3064.0 3064.4 3077.9 3078.9 3091.6 3096.5 3109.9
3132.9 3136.0 3145.5 3156.3 3163.0 3745.4

TS5

-527.1 22.0 40.4 62.9 78.7 83.7 94.6 102.4 127.8
153.9 201.0 235.9 265.6 298.6 331.0 394.8 499.5 591.1
628.1 728.2 775.4 814.8 832.5 896.4 920.6 943.8 973.8
1054.4 1081.1 1094.0 1128.3 1142.7 1157.1 1185.4 1196.8 1224.6
1235.3 1302.9 1312.0 1320.1 1365.3 1383.0 1400.0 1412.6 1423.9
1446.0 1468.9 1486.0 1491.7 1496.1 1500.3 1504.7 1529.7 1644.3
1847.4 3055.7 3059.5 3072.9 3074.8 3075.9 3087.4 3102.3 3120.1
3125.2 3127.6 3145.5 3153.6 3160.2 3800.9

TS6

-785.1 18.3 41.5 68.9 82.2 85.1 100.3 135.5 148.5
167.6 203.1 263.9 297.2 329.4 334.8 395.5 501.0 589.5
725.7 730.2 793.2 809.5 816.0 892.6 911.3 943.1 972.4
1049.9 1081.2 1093.5 1112.5 1139.4 1153.6 1179.4 1185.2 1229.1
1237.3 1297.5 1312.2 1312.5 1329.7 1350.9 1384.2 1401.7 1423.4
1445.2 1450.9 1465.9 1478.1 1485.7 1491.4 1504.4 1506.0 1529.6
1848.1 3035.7 3066.4 3073.9 3076.3 3083.1 3088.1 3095.2 3103.2

TS6'

-718.2 25.2 28.6 39.1 51.1 79.5 95.5 98.2 120.5
155.4 193.4 264.3 288.8 318.5 342.7 392.3 495.3 588.9
705.9 731.6 740.0 809.4 816.3 903.3 934.8 970.5 985.4
1048.8 1073.3 1083.9 1113.1 1136.6 1152.3 1185.2 1218.5 1233.9
1243.2 1293.8 1311.9 1313.2 1329.2 1335.4 1378.8 1399.1 1420.8
1437.2 1444.8 1465.1 1484.5 1491.6 1496.4 1504.4 1507.9 1529.8
1848.9 3058.9 3069.0 3076.2 3077.9 3088.0 3090.5 3091.9 3104.5
3125.0 3128.3 3154.1 3157.9 3160.5 3806.9

(7) $C_3H_7C(O)OC_3H_7$

TS1'

-860.6	25.7	36.7	47.6	57.5	67.4	101.1	101.9	104.5
187.2	193.6	244.8	286.4	326.8	348.6	370.1	500.0	588.0
725.7	745.3	752.1	785.5	888.4	897.0	913.7	925.2	964.0
1055.4	1069.2	1075.8	1087.7	1129.9	1147.6	1182.7	1221.7	1242.1
1254.1	1285.8	1307.8	1322.8	1327.8	1339.9	1357.8	1411.9	1419.7
1426.2	1442.6	1464.9	1477.4	1496.1	1501.8	1506.2	1512.9	1525.5
1851.7	3059.2	3067.9	3072.9	3080.3	3084.6	3093.8	3099.1	3111.6
3115.8	3132.8	3136.7	3140.8	3163.6	3805.7			

TS1

-811.1	29.1	31.5	51.5	78.1	88.2	99.5	112.9	135.9
194.8	198.7	245.8	300.9	322.5	342.0	369.6	512.4	588.5
727.1	736.5	752.3	802.7	870.2	889.4	913.8	934.3	968.6
1052.7	1067.4	1070.4	1117.1	1130.1	1147.4	1176.5	1214.6	1234.6
1254.2	1275.0	1312.0	1327.5	1335.0	1341.3	1349.6	1413.3	1420.0
1434.2	1446.9	1464.8	1475.4	1491.1	1496.0	1506.1	1512.8	1529.7
1850.3	3058.9	3060.5	3067.8	3075.9	3084.4	3095.5	3099.1	3112.0
3115.6	3134.4	3136.5	3140.4	3168.7	3801.4			

TS2

-821.1	31.2	39.9	58.8	79.4	98.2	128.5	135.0	191.8
198.9	226.3	244.6	293.8	316.3	344.5	368.6	505.9	586.3
650.2	727.6	751.9	757.9	889.5	906.7	919.5	937.5	970.3
1017.9	1058.1	1070.6	1108.2	1130.0	1146.6	1168.9	1176.4	1223.1
1255.0	1287.3	1321.6	1329.0	1338.0	1355.3	1411.7	1414.2	1419.9
1436.0	1464.2	1495.2	1495.8	1498.6	1506.4	1510.0	1512.7	1578.1
1860.3	3056.4	3059.8	3064.3	3073.9	3085.0	3097.9	3105.8	3116.1
3122.2	3129.8	3137.3	3142.2	3156.0	3782.8			

TS3

-835.2	36.1	48.6	65.9	89.3	101.9	116.2	137.4	197.7
222.8	244.7	246.1	299.5	337.7	371.2	406.5	513.4	588.9
654.9	727.9	753.2	787.0	888.6	905.3	921.4	951.1	971.5
990.2	1059.2	1070.8	1111.5	1131.8	1154.0	1166.0	1179.0	1246.3
1255.4	1274.5	1318.0	1328.4	1340.3	1353.1	1413.5	1420.2	1421.7
1437.6	1462.8	1491.0	1496.6	1505.5	1506.2	1507.2	1513.4	1513.6
1838.6	3060.2	3062.7	3067.9	3068.2	3084.7	3097.2	3099.9	3114.2
3116.8	3137.4	3140.5	3142.4	3151.4	3761.0			

TS4

-946.5	29.6	56.1	70.0	82.2	85.5	110.9	129.6	184.7
204.2	234.4	251.7	293.5	325.3	338.8	362.1	504.5	598.7
654.5	726.2	764.4	773.9	892.6	896.7	901.7	934.6	967.3
980.6	1049.7	1077.1	1085.3	1122.5	1163.1	1166.5	1190.2	1229.1
1272.3	1282.9	1314.7	1323.1	1325.3	1340.3	1394.0	1419.4	1420.4
1436.3	1483.5	1498.6	1503.8	1506.6	1508.0	1510.5	1511.9	1527.1

1853.7 3062.9 3064.9 3067.3 3069.9 3081.4 3098.2 3104.6 3113.3
3127.4 3136.6 3140.8 3146.1 3148.2 3776.9

TS5

-834.2 24.1 59.6 73.3 87.5 102.1 127.8 158.8 194.7
209.7 232.8 235.4 299.0 338.3 372.4 447.1 507.6 594.2
682.5 735.6 763.0 767.5 897.0 906.1 918.9 946.7 975.8
1047.6 1061.8 1077.5 1094.5 1139.8 1148.8 1164.5 1190.2 1249.2
1256.9 1282.1 1313.3 1325.8 1335.5 1355.1 1407.2 1413.6 1419.7
1439.3 1451.7 1456.2 1495.3 1499.0 1502.4 1506.8 1511.7 1526.5
1827.4 3052.9 3064.1 3064.4 3073.7 3082.2 3099.7 3107.6 3111.5
3124.0 3126.5 3141.7 3147.6 3151.6 3747.6

TS6

-797.9 23.1 38.4 66.5 77.1 84.8 104.2 115.8 136.9
194.1 200.6 236.0 300.6 325.7 347.5 379.7 511.2 593.4
705.9 729.0 763.3 801.8 854.8 897.7 909.2 933.5 974.2
1046.4 1051.2 1080.0 1094.2 1146.5 1164.1 1189.9 1197.3 1238.8
1281.4 1310.8 1324.6 1330.1 1338.4 1350.7 1362.5 1417.1 1418.7
1443.0 1447.7 1468.6 1485.4 1492.7 1498.4 1507.1 1511.5 1526.9
1845.8 3063.4 3064.8 3071.3 3075.8 3079.9 3090.9 3104.9 3105.1
3123.0 3123.4 3139.7 3145.9 3163.5 3804.0

TS6'

-864.6 19.6 49.1 56.8 71.8 73.7 86.7 100.8 103.9
191.8 195.4 233.8 290.4 331.5 351.7 360.0 510.1 590.5
693.8 730.7 756.5 763.6 887.2 898.3 916.2 948.3 975.3
1033.5 1065.7 1077.2 1093.2 1126.1 1163.6 1189.8 1230.6 1240.8
1278.5 1281.4 1318.8 1324.9 1329.9 1336.1 1357.6 1411.2 1419.1
1427.4 1444.3 1465.2 1477.1 1498.4 1503.1 1506.6 1511.5 1526.5
1848.8 3063.9 3071.3 3072.0 3079.7 3080.6 3091.8 3105.2 3105.7
3124.3 3125.6 3140.3 3146.6 3162.0 3804.1

(8) $C_2H_5C(O)OC_4H_9$

TS1'

-804.8 27.8 36.1 43.4 59.0 69.0 94.4 100.3 128.0
175.4 200.9 223.9 266.8 318.1 337.5 425.1 512.7 584.4
679.5 735.5 764.7 815.2 825.9 899.7 930.4 956.6 1011.6
1034.0 1066.4 1074.6 1114.8 1120.7 1126.5 1188.3 1235.8 1249.9
1270.9 1284.8 1288.3 1323.3 1327.9 1342.0 1388.3 1398.2 1423.8
1434.8 1443.8 1468.2 1477.1 1496.7 1498.6 1505.5 1507.0 1526.6
1852.3 3055.7 3066.6 3078.2 3081.0 3082.3 3090.2 3092.2 3108.2
3115.8 3131.0 3157.5 3159.4 3160.3 3805.5

TS1

-770.4 26.7 35.1 51.0 72.3 91.7 95.3 112.0 142.6
177.9 211.2 225.7 282.1 316.0 327.0 440.9 514.4 584.9
679.7 730.1 782.7 814.7 827.1 888.1 926.6 958.7 1018.4
1035.2 1068.5 1094.0 1114.9 1124.8 1128.9 1176.9 1210.3 1246.5

1259.2 1284.1 1295.6 1317.8 1324.9 1345.6 1388.9 1401.2 1423.5
1444.6 1451.2 1468.1 1481.2 1488.1 1498.7 1506.0 1507.0 1526.9
1851.6 3039.3 3061.8 3076.5 3080.9 3082.0 3085.8 3096.2 3108.2
3115.7 3130.5 3157.2 3160.1 3163.1 3803.4

TS2

-554.6 30.4 34.0 52.7 69.2 87.3 108.4 114.9 127.7
168.8 209.3 222.6 242.5 279.8 317.5 435.4 515.5 584.7
636.1 680.0 777.5 816.0 850.4 902.9 939.4 950.4 1021.3
1038.5 1080.9 1089.7 1114.9 1126.0 1157.7 1180.6 1224.9 1245.9
1262.9 1284.5 1290.1 1320.0 1349.8 1384.0 1398.4 1413.1 1423.8
1443.7 1468.0 1488.0 1495.9 1498.8 1500.3 1507.0 1529.2 1556.9
1850.7 3053.4 3057.5 3075.5 3078.3 3080.9 3082.2 3103.8 3116.0
3126.1 3131.9 3149.9 3157.2 3160.2 3795.7

TS3

-775.9 32.7 45.7 58.6 77.5 82.9 108.7 148.2 172.7
209.3 224.5 250.7 278.7 305.7 312.1 437.2 513.0 582.2
658.7 685.4 736.2 810.0 817.9 899.5 942.0 976.7 1016.8
1035.3 1047.5 1078.2 1114.5 1119.7 1126.6 1158.8 1187.9 1236.2
1265.9 1285.8 1297.6 1308.8 1355.3 1383.3 1397.0 1418.9 1423.8
1435.2 1467.0 1485.7 1499.4 1505.5 1506.4 1509.1 1512.2 1572.0
1860.9 3040.7 3064.6 3075.7 3078.1 3082.8 3083.9 3099.5 3113.9
3126.5 3136.9 3145.6 3159.3 3161.8 3781.6

TS4

-831.2 38.4 58.1 64.4 71.5 83.6 138.5 153.0 199.5
215.2 233.2 252.3 284.2 319.1 406.2 425.2 515.6 584.7
660.8 686.5 750.8 815.9 848.3 899.3 938.7 965.1 984.7
1025.8 1043.3 1080.3 1114.0 1116.6 1145.5 1169.0 1176.8 1251.5
1258.9 1285.7 1293.7 1330.8 1333.0 1389.7 1401.4 1418.2 1424.6
1436.6 1465.8 1488.4 1498.8 1500.0 1504.3 1506.3 1509.9 1514.1
1839.6 3048.8 3058.9 3062.3 3081.5 3083.3 3088.3 3099.3 3112.9
3116.5 3132.4 3141.4 3159.8 3161.3 3761.0

TS5

-1003.1 28.1 52.3 65.3 74.8 118.6 127.5 138.3 168.9
207.6 222.5 249.1 276.1 304.7 326.8 437.5 503.6 595.7
641.5 677.6 744.5 810.2 846.2 892.0 924.6 952.6 954.8
1022.7 1060.1 1077.8 1094.5 1098.6 1146.1 1160.5 1192.1 1238.9
1261.4 1295.3 1304.2 1322.4 1331.2 1360.7 1391.6 1415.4 1418.3
1438.9 1486.7 1490.5 1494.2 1499.6 1505.7 1512.2 1523.5 1529.7
1854.4 3051.8 3059.4 3063.0 3073.9 3081.6 3083.0 3102.8 3117.0
3130.8 3135.0 3141.4 3145.5 3166.8 3777.9

TS6

-1170.5 23.4 55.9 62.5 78.6 118.5 124.7 152.0 184.2
213.3 250.8 286.2 312.7 354.5 437.8 450.6 511.3 584.5
665.4 744.0 766.6 811.7 860.0 913.1 939.4 953.3 960.0
1021.1 1044.7 1074.6 1095.9 1102.0 1142.1 1160.6 1192.1 1249.4

1261.4 1270.7 1295.4 1321.9 1323.5 1330.4 1388.6 1408.2 1418.3
1445.3 1448.5 1456.9 1466.5 1494.6 1500.1 1506.1 1512.4 1525.8
1828.3 3052.3 3061.2 3065.1 3074.4 3081.5 3083.2 3105.4 3108.4
3117.9 3130.7 3135.3 3141.1 3189.0 3754.1

TS6'

-825.2 32.3 34.5 43.5 60.8 76.3 90.8 102.6 125.6
182.0 197.2 252.6 278.2 282.4 336.9 437.5 507.2 585.1
669.7 743.7 753.4 810.1 822.7 909.2 952.7 953.3 988.6
1024.7 1064.6 1091.6 1100.6 1114.6 1159.5 1192.1 1211.9 1244.9
1261.0 1279.3 1294.9 1316.5 1322.5 1329.7 1384.2 1393.9 1411.2
1417.8 1444.9 1467.4 1480.9 1494.6 1500.3 1506.2 1512.7 1526.4
1845.1 3051.9 3060.7 3064.5 3078.6 3082.5 3088.7 3103.9 3117.5
3127.3 3128.5 3133.8 3140.2 3187.3 3807.1

(9) $CH_3C(O)OC_5H_{11}$

TS1'

-726.8 25.6 36.5 47.6 51.3 62.0 75.3 89.9 121.6
134.8 199.1 203.1 249.7 328.6 358.8 450.3 493.5 612.8
659.8 715.3 738.7 775.2 859.9 937.6 967.5 988.6 1002.8
1040.8 1071.4 1072.7 1084.8 1109.7 1125.9 1191.9 1224.3 1246.5
1269.8 1301.1 1304.3 1320.1 1329.3 1335.8 1357.8 1399.0 1406.9
1435.9 1444.1 1477.7 1481.7 1482.7 1495.4 1497.0 1509.9 1526.4
1856.3 3042.7 3063.3 3067.2 3075.6 3078.1 3089.1 3089.9 3101.5
3110.7 3130.4 3156.5 3161.3 3202.3 3806.9

TS1

-753.9 26.6 37.1 56.3 61.8 85.7 90.4 98.7 119.8
154.4 199.6 205.5 266.1 324.0 356.5 457.5 497.6 613.2
660.0 720.8 757.7 797.5 864.2 899.7 945.8 984.6 998.5
1044.0 1072.6 1078.9 1090.1 1111.9 1135.4 1179.4 1209.6 1252.6
1279.1 1296.9 1304.0 1324.6 1329.1 1346.0 1359.9 1403.0 1411.9
1444.4 1451.1 1477.4 1480.6 1481.5 1490.1 1496.7 1508.3 1526.4
1856.0 3036.8 3042.1 3063.1 3077.2 3079.4 3088.6 3089.8 3097.3
3107.1 3130.0 3160.7 3161.1 3202.1 3804.0

TS2

-527.6 28.2 39.3 61.9 71.4 84.9 94.5 98.8 117.4
136.7 198.7 204.6 236.9 264.3 353.5 457.4 494.6 613.3
628.1 660.1 754.1 816.4 874.9 913.6 947.6 982.3 999.0
1055.2 1073.1 1082.9 1090.6 1111.7 1159.6 1186.0 1228.2 1246.6
1267.8 1303.1 1316.4 1322.4 1344.8 1351.2 1399.9 1408.6 1412.1
1444.2 1478.0 1482.5 1483.1 1495.1 1500.2 1505.5 1526.2 1597.8
1856.7 3032.0 3055.8 3061.7 3070.7 3077.7 3086.5 3089.8 3107.0
3124.5 3130.7 3147.9 3161.2 3202.3 3798.5

TS3

-533.1 29.3 41.1 57.1 58.4 70.3 80.5 91.7 115.6
138.4 197.2 206.4 251.4 264.8 357.6 456.2 498.1 613.1

632.5 660.4 768.7 785.5 881.8 917.1 948.4 985.7 999.1
1052.3 1072.9 1081.6 1090.9 1116.1 1161.7 1180.7 1218.4 1250.3
1276.7 1300.0 1304.7 1326.7 1337.1 1375.0 1398.6 1406.5 1415.7
1442.6 1477.3 1481.8 1482.9 1493.3 1504.4 1511.1 1528.6 1565.2
1856.4 3043.2 3055.6 3060.6 3063.8 3077.4 3089.8 3090.6 3104.8
3131.8 3132.6 3142.7 3161.3 3202.2 3795.5

TS4

-770.7 41.6 44.0 63.9 70.6 74.2 84.2 133.6 158.8
193.6 207.4 244.6 263.3 302.7 357.8 448.8 485.2 610.3
652.2 682.8 731.5 765.0 869.4 907.6 942.6 995.7 1001.5
1037.4 1065.0 1072.4 1082.0 1106.4 1119.8 1160.7 1188.7 1250.5
1277.4 1292.9 1297.0 1332.3 1348.9 1358.4 1401.7 1409.3 1417.4
1433.5 1477.4 1481.2 1482.7 1497.4 1505.4 1510.6 1512.2 1572.6
1866.3 3027.2 3056.8 3060.3 3072.0 3076.6 3088.2 3094.6 3101.6
3127.4 3130.3 3139.5 3160.0 3202.8 3782.8

TS5

-836.1 41.5 51.3 61.0 73.1 79.1 119.8 143.0 160.2
206.2 224.2 246.9 267.5 348.5 402.0 449.2 497.5 613.2
649.6 678.0 737.6 793.1 888.0 909.7 947.2 979.0 993.2
1008.1 1048.6 1074.1 1088.2 1095.3 1151.6 1174.0 1181.2 1237.1
1270.2 1307.8 1310.9 1327.0 1339.9 1357.0 1403.6 1413.3 1416.7
1434.2 1475.8 1480.7 1487.2 1492.8 1500.8 1503.3 1505.0 1515.0
1845.4 3042.6 3049.9 3055.3 3060.4 3075.1 3090.6 3090.8 3100.5
3114.2 3130.8 3138.0 3162.2 3204.8 3761.4

TS6

-1353.6 35.0 42.2 62.8 71.3 100.0 119.5 135.0 196.8
207.5 246.5 258.1 291.6 345.3 352.8 441.3 488.8 602.6
654.0 737.1 772.1 779.5 861.4 882.7 909.8 948.9 989.3
1031.9 1049.2 1065.8 1089.2 1096.6 1119.5 1161.1 1193.4 1246.6
1254.0 1271.9 1304.8 1308.2 1326.6 1339.2 1354.1 1409.6 1417.2
1436.2 1444.5 1481.8 1491.7 1494.8 1504.5 1505.4 1514.2 1526.2
1856.6 3039.8 3053.4 3059.9 3061.2 3070.1 3082.7 3090.9 3104.9
3130.2 3131.3 3134.6 3138.8 3220.9 3780.4

TS6'

-1502.4 21.2 49.1 53.2 67.9 112.2 127.9 143.7 202.0
206.8 249.5 261.5 296.5 343.8 416.4 440.6 486.2 610.3
647.2 735.7 759.0 772.1 860.4 896.6 911.7 971.1 987.6
1029.8 1049.0 1054.4 1088.8 1091.6 1118.0 1161.2 1192.8 1234.6
1246.1 1271.4 1307.2 1325.8 1332.0 1338.5 1354.0 1408.7 1417.1
1432.9 1455.9 1491.1 1494.5 1495.7 1504.3 1506.1 1513.7 1524.7
1821.7 3038.9 3053.9 3060.2 3065.4 3069.2 3082.7 3091.7 3107.6
3127.8 3130.0 3135.1 3138.5 3212.9 3750.3

(10) $HC(O)OC_6H_{13}$

TS1'

-785.2 32.5 36.0 40.3 66.8 84.9 89.0 96.3 145.6
148.8 165.9 270.3 294.7 339.6 342.0 444.0 474.6 730.1
742.2 767.7 809.8 817.5 901.9 915.1 991.0 1009.8 1031.1
1057.0 1062.5 1084.5 1087.7 1130.2 1191.8 1227.1 1244.9 1259.3
1274.1 1298.6 1310.0 1320.9 1335.7 1338.2 1351.4 1386.0 1408.9
1410.3 1437.2 1443.7 1478.3 1491.9 1492.5 1501.9 1511.0 1524.4
1849.1 3039.6 3045.9 3056.8 3065.7 3069.3 3080.2 3084.3 3088.8
3093.4 3102.2 3109.0 3132.5 3156.6 3805.8

TS1

-748.4 23.6 41.0 57.4 61.0 74.5 88.2 109.1 144.4
160.0 178.1 264.8 320.2 323.5 342.1 447.0 484.3 720.4
744.0 778.3 809.6 822.7 885.0 918.9 991.0 1004.9 1042.1
1062.7 1071.7 1086.4 1096.2 1139.2 1179.5 1204.5 1242.4 1260.5
1263.6 1283.5 1312.6 1325.3 1333.9 1339.8 1346.4 1386.8 1409.8
1415.2 1437.4 1453.4 1480.2 1491.9 1493.1 1499.0 1510.6 1524.3
1848.7 3035.4 3037.8 3045.1 3065.0 3071.1 3080.2 3081.1 3091.2
3092.6 3100.7 3108.3 3132.4 3160.1 3804.3

TS2

-689.2 28.5 41.8 60.5 76.2 76.8 93.0 115.7 143.0
148.7 177.2 236.8 268.1 318.3 341.8 446.3 483.5 622.4
733.8 758.7 809.8 811.8 907.8 918.5 989.7 1001.2 1047.4
1062.5 1077.4 1096.2 1101.5 1151.9 1175.4 1220.5 1252.8 1261.1
1262.5 1294.5 1319.6 1326.3 1339.6 1375.5 1401.0 1410.0 1412.8
1418.8 1437.9 1481.2 1495.8 1499.1 1501.3 1507.2 1524.3 1626.3
1849.0 3030.2 3045.9 3053.1 3063.5 3067.7 3080.9 3082.5 3091.4
3091.6 3108.1 3117.9 3133.5 3137.7 3800.9

TS3

-515.3 29.1 44.0 52.6 67.7 75.0 81.4 93.5 135.4
149.9 175.0 250.4 265.3 320.1 342.1 449.7 481.1 627.1
752.0 772.1 810.0 826.5 909.1 919.2 992.5 1007.8 1047.0
1062.3 1074.3 1092.8 1100.6 1161.2 1187.5 1209.1 1240.5 1260.5
1266.3 1295.1 1313.4 1326.6 1332.9 1366.1 1384.6 1407.9 1409.9
1414.3 1438.6 1480.9 1490.1 1504.1 1506.1 1510.6 1524.5 1601.3
1848.5 3032.9 3043.8 3059.3 3061.9 3065.3 3078.1 3081.2 3092.5
3092.6 3109.8 3130.6 3133.2 3141.3 3797.7

TS4

-538.3 30.8 53.5 56.6 60.0 71.2 87.8 113.2 143.1
155.0 177.1 244.7 266.7 317.8 342.2 443.1 485.5 636.2
741.6 784.9 810.4 824.6 911.8 913.0 992.7 1004.4 1047.2
1062.4 1081.3 1089.8 1094.1 1160.2 1181.3 1203.2 1240.4 1260.2
1272.1 1284.2 1315.1 1322.7 1335.6 1368.8 1386.2 1409.1 1410.4
1416.4 1436.3 1479.7 1492.9 1498.3 1505.2 1512.0 1526.0 1568.6
1849.4 3030.5 3050.8 3056.5 3060.2 3063.8 3076.8 3081.3 3092.5
3095.3 3106.5 3130.3 3137.2 3138.6 3796.4

TS5

-768.1 33.5 52.2 56.6 69.9 93.4 113.6 144.0 151.4
181.6 247.6 264.9 276.2 318.5 342.3 440.9 472.8 674.4
728.4 742.7 800.0 814.3 911.1 916.2 983.8 1016.4 1046.7
1056.6 1059.8 1083.6 1090.9 1119.9 1160.4 1193.5 1239.3 1245.7
1263.4 1291.0 1316.1 1326.3 1337.0 1356.5 1380.8 1409.1 1415.0
1416.1 1426.2 1480.7 1491.2 1501.0 1505.2 1508.4 1513.5 1554.1
1857.1 3028.3 3042.3 3052.5 3060.0 3069.2 3078.1 3078.9 3095.2
3096.5 3102.9 3130.0 3130.3 3137.8 3786.7

TS6

-872.8 36.8 46.5 66.0 84.6 122.9 132.9 140.7 167.2
191.0 247.2 264.8 319.9 335.1 405.3 438.6 483.4 668.3
732.7 760.0 809.3 833.9 910.9 921.1 969.7 1003.8 1011.5
1051.7 1062.6 1072.3 1092.7 1127.9 1164.8 1177.7 1227.8 1255.8
1274.9 1288.3 1314.9 1330.3 1338.3 1340.4 1385.2 1410.9 1415.3
1415.8 1426.0 1473.1 1486.6 1490.4 1495.4 1505.3 1506.8 1515.1
1836.3 3036.2 3045.3 3052.5 3055.1 3059.1 3066.5 3083.6 3094.8
3102.7 3113.1 3116.1 3128.7 3137.0 3765.9

TS7

-826.2 34.0 36.8 50.6 80.8 90.9 97.1 145.0 146.9
175.3 191.5 248.8 264.5 318.8 383.8 444.6 479.6 670.3
731.6 752.1 759.0 807.7 901.5 911.4 936.6 988.6 1010.0
1027.1 1043.5 1071.4 1089.5 1099.4 1159.2 1192.5 1232.6 1234.8
1257.1 1289.9 1320.9 1323.6 1336.3 1338.5 1384.3 1414.8 1416.7
1435.9 1488.8 1490.8 1498.8 1505.7 1506.6 1513.9 1522.5 1704.2
1892.1 3036.8 3043.4 3053.5 3059.7 3064.9 3066.1 3079.2 3084.8
3095.9 3109.8 3129.5 3138.0 3138.8 3794.1

2. Ethers

All frequencies are in cm^{-1}.

（1）$C_3H_7OCH_3$

TS1'

-607.1 54.0 63.0 89.1 112.0 172.2 195.1 236.6 300.2
414.4 450.9 691.5 768.9 905.9 918.3 1017.5 1077.1 1085.5
1161.8 1178.4 1200.1 1245.4 1279.9 1326.0 1334.3 1375.3 1401.1
1417.7 1448.7 1486.4 1498.9 1506.6 1513.0 1529.2 1790.1 3000.2
3032.9 3045.7 3061.6 3078.0 3113.3 3135.8 3144.8 3161.4 3799.1

TS1

-1144.8 27.9 77.0 99.9 130.3 180.2 203.4 234.3 335.8
382.0 427.8 739.5 767.5 904.3 914.8 944.6 1040.3 1080.2
1154.7 1155.7 1192.2 1207.6 1275.8 1291.2 1303.0 1325.8 1339.4
1417.8 1437.2 1493.5 1499.0 1506.5 1512.4 1530.5 1593.7 3006.2
3036.1 3041.9 3062.5 3077.6 3111.1 3113.6 3136.4 3145.2 3794.8

TS2

-397.8 45.9 66.4 67.9 115.2 129.1 192.9 233.0 246.9

417.3 454.0 602.6 773.3 913.5 924.2 1025.0 1073.0 1142.2
1173.4 1183.4 1200.2 1245.7 1262.0 1295.2 1322.7 1406.0 1416.8
1428.4 1488.1 1495.9 1499.4 1506.1 1513.6 1519.1 1932.5 2996.2
3026.0 3060.2 3071.7 3087.0 3112.4 3134.3 3145.7 3168.3 3795.0

TS3

-918.1 83.6 115.5 133.1 151.8 204.7 230.1 237.8 396.9
413.9 447.4 639.1 766.2 918.1 943.3 1003.6 1014.4 1104.3
1152.2 1167.2 1192.8 1199.7 1244.4 1285.6 1325.3 1350.7 1413.3
1428.7 1483.7 1495.1 1498.7 1500.3 1507.9 1523.5 1584.0 2995.6
3026.2 3034.8 3053.4 3082.1 3110.9 3124.4 3153.7 3163.3 3752.9

TS4

-719.6 49.4 62.9 74.6 108.4 145.5 197.1 238.4 324.5
420.7 447.4 676.6 796.2 902.5 930.8 1019.3 1079.8 1116.8
1164.2 1188.6 1202.6 1230.2 1254.6 1295.3 1312.3 1334.3 1356.8
1425.6 1442.9 1483.4 1486.5 1493.3 1499.1 1513.0 1536.1 2991.7
3016.2 3040.9 3062.0 3067.8 3094.8 3118.3 3157.4 3167.0 3804.8

TS4'

-858.8 53.5 69.7 88.6 109.6 125.2 186.3 236.6 339.7
389.2 450.1 708.3 772.6 903.6 939.2 1018.4 1070.6 1080.0
1172.9 1190.8 1197.3 1241.1 1262.8 1285.7 1319.7 1324.5 1357.8
1421.7 1439.6 1476.5 1485.7 1499.3 1503.3 1512.9 1534.3 2992.9
3017.8 3025.7 3069.5 3072.0 3092.0 3118.8 3160.1 3162.5 3805.6

（2）$C_4H_9OCH_3$

TS1'

-606.4 39.6 56.1 74.0 96.9 122.6 141.5 177.0 247.5
301.3 322.6 387.5 501.1 693.5 745.5 819.4 918.4 957.3
1008.2 1061.2 1084.6 1102.0 1160.6 1178.8 1200.4 1241.4 1260.4
1297.6 1324.2 1328.1 1365.8 1396.8 1401.8 1416.4 1449.8 1486.8
1494.5 1500.4 1505.4 1513.0 1529.3 1791.6 3001.4 3032.8 3046.3
3049.5 3061.2 3066.5 3080.7 3113.7 3132.8 3139.3 3161.4 3799.2

TS1

-1143.6 26.9 68.1 72.4 110.8 140.1 142.4 217.5 245.5
288.8 338.5 384.9 469.1 743.2 745.2 817.0 918.1 939.1
956.8 1040.2 1065.1 1092.9 1154.2 1155.8 1194.3 1206.8 1257.2
1290.6 1290.8 1308.4 1323.2 1328.5 1391.4 1417.4 1439.0 1493.5
1494.3 1500.3 1504.9 1513.1 1530.6 1595.5 3007.5 3035.8 3043.0
3050.3 3060.9 3066.1 3081.3 3110.7 3113.3 3132.6 3139.5 3794.8

TS2

-398.4 43.4 55.9 79.0 97.7 123.9 135.6 154.4 235.4
252.0 320.0 388.9 504.5 603.1 747.9 828.4 918.5 960.0
1023.1 1060.8 1087.8 1145.2 1173.1 1185.4 1200.9 1240.9 1252.7
1283.8 1290.9 1326.9 1381.8 1409.8 1417.0 1430.7 1486.4 1494.5
1499.4 1500.7 1505.7 1514.3 1518.5 1932.8 2998.1 3026.2 3046.9
3059.0 3061.8 3082.2 3087.2 3111.5 3132.3 3139.1 3168.2 3794.9

TS3

-873.0	66.7	84.9	107.2	115.3	140.9	181.2	231.8	253.9
321.3	382.2	406.8	493.7	660.1	738.5	822.4	926.4	980.2
1003.8	1032.3	1058.8	1123.1	1142.3	1176.0	1193.6	1198.9	1239.9
1265.3	1299.2	1306.8	1351.5	1386.9	1417.9	1429.5	1483.2	1485.7
1499.7	1505.3	1508.1	1510.0	1523.8	1576.7	2997.4	3025.8	3035.9
3037.0	3064.0	3081.5	3082.0	3104.2	3136.3	3143.9	3162.7	3752.0

TS4

-517.2	48.4	57.8	78.0	95.8	123.6	138.3	145.7	229.9
245.0	317.9	389.5	497.5	631.6	792.6	827.9	914.1	964.0
1012.3	1063.0	1095.5	1146.1	1176.0	1197.2	1202.8	1210.8	1244.5
1262.8	1293.5	1321.1	1351.3	1387.7	1412.8	1440.7	1485.2	1488.7
1496.5	1498.8	1500.7	1513.6	1536.6	1620.2	2991.6	3015.6	3039.9
3054.3	3057.4	3066.9	3076.6	3108.4	3125.0	3144.8	3156.7	3801.2

TS5

-770.8	47.5	59.1	95.9	125.3	128.6	143.2	160.9	238.9
322.3	328.4	388.9	499.8	738.3	795.4	820.1	903.3	952.5
1010.2	1058.5	1093.3	1114.2	1167.9	1183.9	1203.1	1206.9	1246.8
1250.1	1297.8	1316.9	1323.5	1354.1	1394.3	1439.8	1451.3	1480.0
1486.6	1487.9	1499.7	1504.2	1513.4	1534.6	2989.9	3016.0	3021.8
3036.7	3063.1	3067.0	3083.6	3095.3	3116.5	3158.4	3161.7	3801.8

TS5'

-718.4	41.6	49.2	74.3	80.6	117.4	139.1	147.3	237.5
289.3	342.1	388.0	495.2	718.5	750.5	821.0	946.4	978.7
1009.9	1059.4	1076.7	1107.8	1177.6	1191.7	1201.1	1233.3	1248.3
1259.0	1290.7	1320.1	1322.6	1335.2	1386.2	1437.5	1441.4	1484.5
1486.6	1499.4	1499.6	1505.7	1513.6	1534.5	2991.3	3016.1	3023.3
3059.3	3067.0	3069.6	3090.2	3094.0	3118.6	3157.7	3158.3	3807.2

（3）$C_5H_{11}OCH_3$

TS1'

-606.6	32.8	43.1	60.2	77.3	108.0	113.3	135.6	181.4
246.0	263.2	302.6	318.3	435.3	518.3	694.6	734.9	775.8
866.9	909.3	989.8	1016.4	1039.8	1078.2	1089.5	1106.3	1161.1
1178.3	1199.9	1238.1	1245.9	1276.1	1307.3	1324.4	1338.0	1348.2
1372.9	1402.1	1410.8	1415.3	1449.8	1486.7	1490.5	1494.0	1504.3
1505.1	1513.7	1529.1	1791.9	3001.7	3032.9	3035.7	3046.4	3054.7
3059.3	3065.8	3067.5	3092.5	3115.3	3129.4	3137.0	3161.3	3799.2

TS1

-1142.0	24.4	60.1	62.3	84.6	113.6	125.0	155.7	216.3
244.0	244.9	311.7	338.0	408.5	501.1	735.3	742.6	775.4
865.5	911.4	938.6	989.6	1036.7	1057.6	1085.0	1089.1	1156.2
1156.4	1194.8	1206.0	1243.2	1269.3	1290.4	1305.3	1307.3	1324.1
1338.0	1353.4	1408.7	1416.1	1438.9	1490.8	1493.5	1494.3	1504.4
1505.2	1514.0	1530.3	1595.5	3007.8	3035.6	3036.8	3043.3	3053.8

3059.3 3066.3 3066.8 3091.7 3110.6 3114.9 3129.2 3137.3 3794.7

TS2

-399.3 37.5 46.7 66.3 95.4 106.0 113.8 141.9 148.4
239.8 247.0 260.8 318.8 437.7 520.1 607.2 737.1 779.4
873.6 910.2 990.0 1026.9 1046.5 1080.2 1088.7 1148.9 1172.5
1186.1 1200.3 1236.8 1244.8 1269.8 1279.3 1314.1 1335.5 1345.6
1398.3 1412.7 1415.8 1430.9 1486.1 1492.1 1494.4 1499.9 1504.2
1505.0 1514.5 1518.6 1930.7 2998.8 3026.6 3033.1 3053.7 3058.5
3059.8 3068.3 3087.6 3092.0 3112.9 3128.5 3136.8 3168.3 3794.7

TS3

-872.1 58.6 67.9 84.2 91.8 125.8 157.6 171.2 233.3
245.9 272.9 318.9 407.5 432.2 497.1 674.7 732.3 773.2
879.0 910.0 1002.7 1009.0 1022.3 1050.1 1085.1 1119.1 1149.4
1177.1 1193.5 1197.8 1236.0 1252.4 1279.7 1295.0 1331.6 1348.5
1354.4 1406.3 1416.4 1429.7 1481.4 1483.9 1497.5 1499.7 1505.4
1508.2 1512.0 1523.6 1576.3 2997.6 3022.9 3025.9 3036.6 3056.6
3059.5 3069.7 3081.5 3095.9 3105.3 3129.1 3138.3 3162.6 3752.0

TS4

-498.1 46.0 56.3 67.1 87.4 104.4 120.7 131.6 163.0
238.8 251.9 264.3 318.0 437.2 514.0 625.4 763.0 796.1
886.4 911.8 988.4 1018.2 1044.9 1084.7 1097.5 1147.3 1177.5
1197.1 1200.0 1216.3 1240.4 1256.7 1282.5 1301.4 1314.3 1326.6
1360.1 1401.0 1412.7 1440.5 1482.4 1486.3 1493.1 1499.6 1504.3
1510.5 1513.2 1535.9 1638.5 2991.7 3015.7 3037.0 3044.8 3056.7
3058.1 3061.3 3067.1 3091.6 3110.0 3129.2 3140.1 3157.1 3798.4

TS5

-531.0 41.7 52.7 75.3 104.6 109.3 124.0 140.8 149.2
232.3 240.5 266.2 316.9 432.5 516.9 633.2 750.6 808.7
880.0 917.7 984.5 1017.6 1046.6 1087.8 1096.7 1143.8 1176.5
1195.4 1201.8 1238.4 1243.4 1248.8 1276.0 1314.7 1319.2 1338.0
1348.6 1403.3 1411.0 1440.0 1482.5 1486.4 1494.8 1499.8 1500.0
1503.9 1513.1 1534.2 1591.7 2990.2 3015.8 3022.2 3029.3 3054.7
3062.9 3066.7 3069.9 3086.0 3114.6 3123.4 3147.3 3158.0 3797.0

TS6

-742.7 42.1 48.5 74.6 94.6 110.3 113.7 133.5 162.3
239.1 264.7 318.0 322.3 436.0 518.1 725.4 763.0 800.8
867.5 901.4 986.3 1016.4 1038.8 1084.5 1089.9 1124.4 1173.8
1184.2 1201.9 1208.2 1241.4 1244.8 1280.7 1297.0 1323.7 1327.8
1349.3 1360.4 1409.1 1440.5 1458.3 1481.9 1486.1 1496.2 1499.1
1503.3 1508.4 1514.1 1534.4 2988.5 3014.8 3020.1 3034.7 3040.3
3065.2 3065.3 3075.5 3087.5 3098.3 3115.0 3157.3 3158.9 3804.6

TS6'

-794.7 36.9 51.2 68.8 89.4 95.8 116.4 137.5 146.9
239.1 249.0 309.0 340.7 428.5 510.7 724.0 741.3 780.9
867.6 928.4 990.7 1008.2 1032.1 1070.5 1086.8 1109.9 1178.2

1196.9 1199.6 1232.7 1239.6 1267.8 1290.9 1313.3 1324.6 1330.2
1337.1 1371.0 1401.8 1439.3 1441.8 1477.8 1486.2 1494.5 1496.6
1499.6 1509.0 1514.0 1534.3 2989.2 3015.6 3020.4 3040.4 3054.0
3066.4 3067.0 3072.9 3088.7 3098.3 3116.2 3157.5 3158.2 3806.0

（4） $C_6H_{13}OCH_3$

TS1'

-1137.4 18.8 48.6 53.0 76.8 98.0 104.1 142.6 154.3
194.2 209.8 245.2 285.5 332.2 337.1 466.0 494.0 731.1
742.4 753.3 812.8 905.6 911.2 938.7 1011.2 1022.0 1060.3
1071.0 1087.7 1096.6 1156.2 1157.1 1195.2 1205.8 1233.7 1255.6
1286.6 1293.2 1305.2 1320.7 1324.7 1334.4 1338.0 1384.9 1414.4
1416.6 1439.2 1488.6 1490.3 1493.9 1498.3 1504.8 1506.9 1514.2
1530.3 1594.5 3007.7 3035.1 3035.9 3041.0 3043.2 3052.3 3059.0
3062.7 3066.3 3076.4 3094.8 3110.6 3115.4 3128.8 3136.4 3794.8

TS1

-606.4 28.7 41.1 62.6 71.4 88.0 96.2 124.8 144.6
181.4 207.9 246.3 284.8 302.1 360.7 479.7 510.6 693.9
731.0 753.6 813.3 906.4 910.9 1002.9 1011.3 1047.0 1060.9
1084.7 1091.8 1111.7 1161.6 1178.4 1199.9 1235.0 1236.2 1263.8
1289.8 1320.8 1322.6 1334.1 1337.7 1364.9 1389.5 1402.3 1414.2
1416.6 1449.7 1486.8 1488.4 1490.5 1498.3 1504.7 1507.0 1514.2
1529.2 1792.4 3001.6 3032.8 3034.7 3040.4 3046.3 3051.8 3058.6
3062.2 3067.0 3075.8 3094.5 3115.7 3128.4 3135.7 3161.3 3799.2

TS2

-398.9 34.6 36.8 53.9 84.2 95.7 110.0 112.2 140.9
156.6 205.9 240.0 247.8 285.6 359.6 481.9 512.6 605.9
732.3 755.3 818.6 909.7 911.7 1010.6 1011.3 1052.4 1068.3
1083.8 1093.6 1151.0 1172.4 1186.4 1200.3 1232.7 1236.1 1261.1
1273.8 1297.7 1317.1 1333.0 1335.0 1376.6 1406.3 1414.0 1416.0
1430.7 1485.6 1489.8 1491.9 1497.1 1499.8 1505.2 1507.3 1514.7
1518.6 1931.5 2998.7 3026.6 3032.9 3039.7 3051.5 3058.7 3059.5
3064.3 3076.4 3087.6 3094.7 3113.4 3128.6 3136.0 3168.2 3794.8

TS3

-871.4 41.5 62.0 73.5 84.3 115.2 127.9 153.5 165.0
221.0 233.6 249.1 287.7 354.1 405.3 472.8 494.6 673.2
730.3 750.3 815.6 911.6 921.5 998.2 1018.4 1025.9 1048.8
1068.1 1090.6 1121.6 1151.3 1178.4 1193.9 1197.8 1232.4 1241.8
1265.4 1288.3 1315.9 1325.6 1336.1 1352.1 1381.4 1414.8 1416.1
1429.7 1480.9 1484.1 1491.5 1499.8 1501.3 1505.2 1508.3 1513.7
1523.6 1577.3 2997.6 3023.8 3025.9 3036.4 3041.8 3051.5 3059.4
3067.3 3076.8 3081.4 3096.8 3105.6 3129.6 3136.6 3162.6 3752.1

TS4

-499.5 42.8 54.5 60.7 63.1 79.9 104.2 113.4 148.3
169.7 208.5 237.4 245.6 285.9 355.6 482.1 506.1 627.1

740.9 794.8 819.1 911.7 919.2 1002.7 1009.0 1048.6 1072.5
1088.1 1098.9 1150.0 1178.0 1197.6 1198.2 1214.4 1234.4 1254.2
1276.7 1282.2 1306.7 1319.5 1328.4 1343.7 1381.0 1408.7 1415.9
1440.4 1479.9 1485.9 1492.0 1498.4 1498.9 1504.8 1512.0 1513.5
1535.6 1636.1 2992.0 3015.8 3030.9 3037.2 3048.4 3056.6 3059.9
3061.2 3067.1 3075.1 3094.0 3110.2 3130.1 3137.6 3156.9 3798.3

TS5

-515.0 42.1 44.5 58.7 81.5 83.4 111.1 128.9 133.6
161.3 207.1 237.4 252.7 285.2 361.4 481.2 509.5 630.7
748.8 776.4 820.4 910.9 928.0 1004.7 1009.8 1050.8 1064.0
1090.5 1100.2 1149.0 1176.5 1194.4 1201.5 1226.0 1234.4 1247.0
1270.4 1294.0 1312.5 1324.8 1329.6 1355.3 1384.1 1407.6 1416.3
1440.0 1480.1 1485.8 1489.8 1498.9 1503.4 1504.6 1511.3 1513.3
1534.1 1604.4 2989.9 3015.6 3021.9 3030.3 3041.4 3060.5 3061.7
3063.4 3066.4 3077.6 3090.3 3114.4 3132.3 3142.2 3157.6 3797.0

TS6

-506.7 36.0 43.4 60.9 80.8 89.3 101.2 111.8 143.1
150.4 206.3 237.9 242.3 286.2 356.8 478.8 509.4 621.9
742.0 785.7 847.1 908.7 916.9 1003.7 1006.8 1052.6 1067.2
1091.5 1094.2 1147.5 1178.5 1197.8 1201.5 1230.2 1234.4 1235.8
1265.4 1295.6 1319.1 1320.0 1329.6 1339.5 1378.9 1409.9 1412.6
1440.4 1480.9 1485.9 1495.3 1495.6 1499.6 1500.6 1507.1 1513.7
1534.1 1639.1 2988.3 3014.7 3019.8 3030.1 3037.5 3055.3 3064.7
3065.0 3067.4 3075.7 3090.7 3114.5 3123.8 3146.6 3157.3 3799.9

TS7

-749.8 33.2 42.7 65.3 86.9 97.0 114.4 126.2 148.7
163.9 208.6 240.1 286.2 322.2 360.3 481.7 508.9 727.5
749.3 788.0 819.2 887.4 917.7 1002.5 1005.7 1045.9 1064.3
1086.2 1094.9 1129.9 1174.3 1182.8 1201.6 1206.5 1233.4 1238.8
1269.4 1280.6 1313.2 1324.0 1332.8 1338.2 1352.7 1387.7 1414.0
1440.5 1456.3 1480.3 1486.1 1492.0 1495.3 1499.0 1499.6 1509.8
1514.3 1534.3 2988.9 3014.3 3020.1 3034.2 3035.7 3043.2 3064.0
3065.1 3067.6 3079.6 3090.0 3100.2 3113.7 3157.3 3159.0 3803.4

TS7'

-775.5 33.9 42.1 52.2 73.1 87.0 101.5 110.8 145.4
153.6 196.6 239.7 280.8 327.0 358.8 469.5 509.5 728.6
739.4 765.1 819.4 904.9 919.7 1003.4 1011.3 1031.9 1055.1
1083.3 1087.7 1117.6 1179.0 1196.6 1200.2 1227.0 1233.2 1259.4
1277.3 1301.1 1311.9 1319.5 1333.8 1337.1 1354.7 1387.0 1409.2
1440.4 1451.8 1479.8 1485.9 1491.7 1494.0 1499.5 1502.0 1510.3
1514.3 1534.3 2988.8 3015.2 3019.9 3037.2 3044.2 3054.8 3065.7
3066.0 3066.8 3082.1 3088.4 3102.0 3114.9 3156.2 3157.7 3806.1

（5） $C_5H_{11}OC_2H_5$

TS1'

-890.2 28.5 41.2 49.3 80.1 84.7 107.8 110.7 133.2
168.7 194.2 243.3 285.7 327.4 361.2 489.9 501.1 734.8
767.5 775.0 832.5 866.5 905.1 919.9 989.9 1026.2 1052.7
1059.7 1088.8 1093.1 1154.1 1180.8 1189.5 1200.6 1226.4 1244.1
1271.3 1292.7 1303.8 1309.9 1323.0 1337.7 1350.8 1398.0 1402.6
1413.0 1415.2 1454.5 1485.8 1490.7 1493.8 1503.7 1504.2 1513.4
1521.8 1537.2 2995.4 3018.0 3027.8 3035.6 3052.2 3053.1 3058.5
3065.3 3065.5 3090.6 3110.5 3113.0 3128.3 3136.0 3183.9 3808.4

TS1

-1218.0 33.1 41.2 72.4 96.2 104.6 138.4 164.0 175.7
213.9 247.6 291.3 353.1 362.7 423.8 493.7 500.5 706.5
734.5 774.2 863.5 874.7 912.9 929.8 974.3 991.0 1044.0
1068.4 1088.4 1091.3 1148.9 1163.8 1190.4 1195.8 1210.9 1243.8
1271.8 1280.6 1307.2 1315.5 1324.7 1338.2 1351.8 1398.4 1413.0
1416.0 1446.7 1463.4 1490.3 1493.4 1503.4 1505.5 1511.0 1514.6
1525.4 1535.8 3001.5 3008.2 3036.5 3038.3 3046.9 3053.5 3059.1
3062.6 3066.7 3091.2 3111.5 3114.3 3128.9 3137.4 3191.7 3753.2

TS2

-419.5 36.2 39.1 60.6 85.1 100.3 105.6 117.5 130.7
173.7 205.2 245.1 250.1 295.1 354.4 499.7 504.9 600.7
735.2 775.8 858.4 871.1 906.3 930.4 990.2 1043.1 1060.5
1088.2 1091.5 1135.1 1156.3 1176.8 1197.0 1201.4 1245.0 1265.0
1271.7 1307.6 1324.0 1338.0 1350.3 1373.9 1392.4 1412.0 1415.4
1417.5 1462.0 1485.1 1490.9 1494.1 1502.7 1504.4 1504.8 1514.0
1529.8 1904.5 2998.7 3012.7 3035.3 3039.9 3053.5 3058.6 3065.3
3067.0 3073.5 3091.2 3114.7 3128.4 3136.3 3149.8 3161.9 3796.8

TS3

-396.3 36.0 43.6 50.5 68.6 82.7 105.9 117.2 135.8
173.3 204.5 245.6 254.5 294.9 357.0 497.4 504.8 605.8
736.5 778.4 824.3 873.9 903.1 923.8 989.9 1043.6 1066.6
1088.1 1091.3 1135.0 1172.1 1183.2 1192.1 1200.3 1244.5 1265.0
1277.9 1313.8 1316.5 1335.1 1344.8 1387.5 1398.2 1411.7 1415.5
1417.7 1465.3 1489.4 1489.5 1492.5 1503.4 1505.0 1506.6 1514.3
1534.5 1936.7 2999.6 3016.6 3032.9 3053.4 3058.4 3058.5 3059.5
3068.4 3074.9 3091.8 3112.5 3128.4 3136.6 3152.3 3156.8 3794.9

TS4

-874.8 43.7 62.2 67.9 78.1 88.8 145.1 163.3 173.6
210.6 245.3 256.0 296.3 356.7 407.7 477.8 501.8 672.7
732.4 773.1 824.0 879.4 902.3 923.8 1002.8 1020.4 1050.9
1060.8 1087.6 1118.5 1141.0 1175.4 1179.2 1194.3 1199.5 1249.8
1276.1 1292.5 1313.5 1331.3 1347.8 1352.5 1392.1 1406.7 1416.2
1417.4 1456.7 1481.5 1490.6 1497.4 1504.8 1505.4 1511.2 1512.5
1536.4 1577.7 2998.2 3016.4 3022.8 3037.4 3049.2 3056.6 3059.4
3069.5 3073.8 3095.8 3104.9 3129.0 3138.2 3151.0 3155.6 3748.3

TS5

-497.1 40.7 44.2 56.6 81.3 87.3 108.8 119.2 128.9
173.7 204.8 252.4 255.2 294.2 358.6 497.1 503.7 625.0
762.9 794.1 824.9 886.0 904.4 925.0 988.3 1045.2 1062.8
1091.1 1097.4 1135.4 1178.7 1182.0 1197.4 1206.6 1217.8 1252.0
1278.0 1300.5 1311.1 1314.6 1326.6 1358.7 1392.6 1401.7 1412.6
1420.5 1463.9 1482.8 1488.9 1492.5 1504.1 1506.0 1510.4 1523.9
1541.8 1639.9 2992.2 3005.6 3035.3 3038.3 3044.8 3056.4 3058.1
3061.0 3073.5 3091.4 3109.6 3129.1 3139.9 3150.8 3154.8 3798.4

TS6

-529.9 32.9 44.9 63.6 90.4 93.8 115.8 120.0 152.8
165.7 204.2 238.7 252.5 294.8 353.6 499.5 503.1 635.6
750.0 807.4 825.1 880.5 907.0 928.1 984.6 1047.2 1063.0
1092.8 1097.5 1133.2 1176.6 1183.2 1196.2 1206.6 1242.7 1249.1
1268.0 1308.8 1315.4 1320.0 1337.4 1346.1 1392.0 1404.0 1411.2
1420.8 1463.6 1482.7 1488.3 1495.3 1500.4 1503.3 1506.3 1522.9
1540.8 1594.5 2990.8 3005.7 3023.4 3029.2 3034.7 3054.8 3062.6
3069.7 3073.8 3085.8 3114.2 3123.4 3147.3 3151.2 3155.2 3797.2

TS7

-743.3 29.7 42.5 66.7 82.6 88.5 94.3 124.6 139.9
173.4 206.8 254.0 294.6 320.9 357.5 501.8 503.3 725.8
762.9 799.6 823.9 867.0 898.5 919.5 986.3 1039.4 1060.3
1089.7 1091.5 1119.1 1163.4 1180.9 1192.3 1207.0 1208.6 1242.6
1274.9 1295.4 1310.7 1323.6 1327.6 1349.8 1357.5 1393.7 1408.2
1421.2 1458.5 1463.6 1481.8 1488.7 1495.7 1503.3 1505.5 1509.0
1523.2 1540.7 2989.1 3004.6 3021.3 3033.4 3034.5 3040.2 3064.9
3073.8 3075.1 3087.4 3098.2 3114.6 3151.1 3155.2 3158.8 3804.4

TS7'

-793.5 35.0 43.5 47.4 72.5 86.3 100.5 112.2 133.5
167.5 194.6 252.3 290.3 328.9 354.0 490.5 503.3 722.4
740.4 779.8 823.3 868.0 910.8 933.3 990.6 1026.5 1053.3
1079.6 1089.1 1107.3 1170.5 1179.7 1198.7 1206.4 1237.3 1258.1
1290.2 1308.8 1315.4 1324.5 1328.7 1336.8 1369.6 1392.8 1402.4
1420.2 1442.0 1463.7 1478.1 1488.3 1494.4 1496.5 1505.5 1509.9
1523.3 1541.0 2989.7 3005.3 3021.6 3034.3 3040.3 3053.6 3066.6
3072.8 3073.9 3088.7 3098.2 3115.8 3151.3 3155.3 3157.5 3805.9

（6）$C_4H_9OC_3H_7$

TS1'

-854.5 33.7 46.2 48.5 78.8 86.1 100.7 107.9 137.2
169.0 194.9 246.1 287.1 333.1 348.2 493.0 499.4 710.2
743.9 771.5 817.5 903.2 917.9 945.1 957.8 1029.9 1058.1
1079.1 1086.5 1097.0 1164.6 1178.4 1197.7 1203.8 1254.9 1263.6
1281.6 1295.9 1318.5 1321.0 1325.9 1327.8 1356.4 1388.8 1414.7
1416.8 1429.7 1464.0 1476.8 1493.8 1499.5 1503.8 1504.8 1512.4
1521.6 1538.4 2990.3 2998.5 3025.2 3027.4 3049.1 3060.0 3065.1

3071.6 3079.6 3091.8 3111.3 3118.4 3131.5 3137.8 3162.2 3805.6

TS1

-718.4 29.8 39.8 62.7 69.9 84.9 94.2 123.2 134.1
177.5 205.5 249.7 295.1 324.3 352.3 493.6 511.1 680.1
744.1 796.2 818.3 901.7 920.6 931.9 957.8 1037.7 1060.1
1084.2 1092.8 1122.5 1159.8 1182.2 1194.9 1205.8 1233.5 1259.1
1290.8 1296.2 1310.1 1322.1 1327.1 1334.1 1353.8 1388.7 1415.8
1418.5 1432.6 1465.9 1484.6 1493.2 1494.6 1500.0 1505.4 1512.6
1523.0 1540.1 2989.5 2996.7 3024.6 3042.1 3048.9 3059.4 3061.8
3064.5 3079.3 3094.5 3110.6 3117.8 3130.9 3137.0 3166.4 3805.1

TS2

-921.0 36.6 45.1 75.0 107.6 121.0 133.4 156.7 174.7
207.6 233.7 249.7 290.4 348.1 414.1 492.8 505.5 639.3
744.0 766.4 817.5 913.8 923.8 944.3 959.3 1007.6 1034.7
1059.4 1092.8 1111.0 1148.2 1168.5 1184.3 1195.1 1196.7 1258.0
1285.0 1294.3 1322.7 1324.7 1328.8 1349.1 1388.4 1412.5 1414.3
1417.2 1458.7 1493.6 1495.0 1499.2 1499.5 1505.7 1509.6 1514.0
1533.0 1584.8 2995.4 3005.3 3035.4 3038.1 3049.7 3053.1 3060.1
3063.1 3080.7 3109.8 3110.5 3124.1 3132.3 3139.3 3153.4 3748.4

TS3

-393.0 34.8 44.1 49.4 75.0 83.4 89.2 112.1 134.9
178.7 200.6 239.0 248.4 295.5 352.6 496.8 506.4 603.3
744.4 773.7 818.3 912.3 918.6 929.0 957.7 1037.8 1057.1
1081.0 1095.2 1140.3 1166.5 1184.8 1197.9 1200.7 1253.9 1265.6
1292.0 1296.9 1321.3 1326.4 1328.8 1385.3 1406.2 1409.6 1416.5
1417.8 1466.4 1493.3 1494.6 1500.4 1505.0 1505.9 1513.0 1513.9
1531.1 1942.1 2996.5 3004.2 3045.4 3049.5 3059.9 3060.1 3065.5
3071.4 3080.6 3112.1 3112.3 3131.5 3134.0 3137.7 3145.3 3795.6

TS4

-395.0 38.9 45.8 51.4 58.0 80.5 105.6 114.5 145.0
176.9 206.4 236.9 247.2 295.6 345.7 497.2 507.8 604.9
746.6 767.4 827.6 904.5 913.3 927.3 960.7 1041.9 1055.7
1084.7 1089.5 1140.7 1167.4 1185.3 1196.8 1200.6 1250.5 1280.1
1280.8 1290.5 1326.2 1328.0 1336.2 1380.9 1405.0 1412.3 1416.6
1417.3 1466.6 1490.5 1498.7 1500.0 1505.0 1506.7 1512.8 1513.8
1530.7 1939.7 2997.9 3003.9 3044.9 3046.8 3058.5 3061.4 3061.5
3076.8 3082.3 3110.9 3112.3 3132.0 3135.2 3138.6 3143.3 3795.3

TS5

-878.8 41.9 49.4 77.2 78.8 118.9 125.8 153.5 180.5
208.2 236.9 253.2 290.9 349.3 414.1 490.9 508.6 658.6
739.7 766.7 822.8 905.9 916.9 933.2 981.2 1020.7 1042.2
1055.8 1079.8 1124.5 1139.7 1176.4 1183.6 1194.8 1196.4 1262.7
1280.5 1295.0 1306.6 1326.0 1336.5 1351.3 1384.8 1412.7 1418.2
1418.4 1458.2 1485.7 1497.6 1505.2 1507.1 1508.9 1510.3 1513.7
1533.1 1577.6 2996.7 3004.4 3035.6 3036.5 3038.0 3062.3 3063.9

3073.3 3081.8 3103.9 3110.6 3134.7 3136.1 3143.7 3145.2 3747.8

TS6

-515.7 27.4 38.4 49.9 60.1 86.7 98.9 114.1 135.7
166.4 202.9 235.7 240.5 295.8 346.0 493.6 508.3 627.6
766.3 790.8 826.3 904.8 910.6 924.9 964.8 1038.2 1057.7
1083.5 1096.4 1142.6 1179.8 1186.3 1197.3 1205.3 1212.0 1261.8
1278.9 1287.4 1319.0 1325.7 1335.5 1351.1 1386.3 1412.6 1416.5
1419.1 1465.5 1487.5 1496.2 1498.1 1500.4 1506.8 1511.7 1522.8
1539.9 1621.0 2988.2 2996.2 3022.4 3040.9 3054.1 3057.2 3060.5
3075.8 3076.4 3107.9 3110.6 3124.8 3133.8 3141.8 3144.4 3800.9

TS7

-769.5 32.0 38.6 65.1 85.8 93.1 116.2 125.8 158.5
166.7 205.0 236.5 295.9 325.8 349.8 494.5 509.8 737.8
766.6 792.4 819.0 900.4 906.5 922.6 953.4 1033.9 1055.0
1082.1 1094.2 1116.7 1160.1 1184.0 1193.0 1202.3 1211.0 1248.2
1278.4 1293.4 1315.1 1320.9 1326.6 1336.3 1354.7 1391.4 1416.9
1419.3 1452.0 1465.0 1481.2 1488.5 1497.9 1504.3 1506.9 1511.8
1521.9 1538.7 2987.2 2995.7 3021.7 3023.9 3036.6 3060.8 3062.7
3076.2 3083.6 3095.2 3111.1 3115.9 3134.2 3142.5 3161.5 3801.7

TS7'

-715.7 29.3 39.0 49.4 67.9 84.2 95.0 109.7 139.3
168.4 199.9 236.7 280.9 326.2 352.4 487.5 510.3 717.2
749.5 766.4 820.3 904.4 919.8 947.4 981.6 1030.6 1055.0
1075.9 1086.0 1110.6 1170.1 1182.8 1200.1 1203.4 1240.2 1257.8
1278.2 1285.5 1318.1 1321.7 1325.2 1332.4 1337.9 1384.3 1416.2
1417.3 1440.9 1464.3 1485.6 1497.9 1499.9 1506.0 1506.7 1511.9
1522.2 1538.7 2987.9 2996.6 3021.8 3025.2 3059.1 3060.8 3069.2
3076.2 3090.0 3093.8 3111.0 3118.2 3134.1 3142.4 3157.4 3807.2

3. Ketones

All frequencies are in cm^{-1}.

（1）$CH_3C(O)C_2H_5$

TS1

-1463.0 33.6 83.8 148.1 210.2 256.4 278.7 366.1 429.7
479.6 586.0 709.4 752.5 819.8 901.1 951.1 1007.0 1014.6
1118.8 1124.6 1217.3 1229.7 1286.5 1381.1 1419.3 1433.9 1456.1
1481.5 1497.3 1504.4 1824.8 3054.8 3081.9 3086.6 3105.5 3157.5
3161.5 3180.8 3743.9

TS2

-621.1 40.8 51.5 72.5 104.0 143.7 203.1 251.7 404.9
478.2 590.3 657.5 778.8 782.5 951.1 974.0 1003.9 1091.6
1133.7 1153.9 1196.2 1286.0 1361.7 1399.3 1415.9 1472.6 1478.7
1487.1 1492.6 1546.6 1843.9 3067.6 3073.5 3094.9 3136.0 3142.5
3163.6 3186.4 3799.1

TS3

-1151.1 52.6 107.3 125.0 160.8 245.9 345.9 401.9 455.2
472.6 598.7 721.0 760.3 856.1 927.0 972.4 976.5 1036.4
1121.7 1137.3 1202.6 1257.9 1318.0 1379.7 1406.5 1439.4 1450.9
1463.7 1469.9 1482.0 1839.3 3047.1 3069.5 3081.9 3113.7 3137.6
3186.9 3187.5 3758.7

TS3'

-788.9 40.4 56.3 72.4 96.1 104.4 220.5 320.0 397.3
474.5 595.5 704.4 754.6 827.4 937.9 952.5 1017.4 1084.5
1132.4 1194.5 1224.7 1280.3 1316.3 1368.1 1394.5 1413.9 1459.4
1471.3 1480.1 1481.9 1848.0 3062.3 3070.3 3099.3 3116.5 3137.8
3184.5 3185.3 3806.6

（2）$CH_3C(O)C_3H_7$

TS1

-1461.8 29.0 71.8 99.3 126.1 198.0 245.2 275.5 333.4
372.8 433.3 482.4 584.6 716.6 742.6 829.6 859.1 905.9
931.6 976.3 1017.1 1071.5 1134.8 1141.5 1211.1 1226.9 1258.4
1324.7 1331.2 1406.3 1418.7 1433.0 1453.4 1481.0 1494.6 1505.9
1511.3 1823.6 3041.7 3059.2 3072.8 3084.2 3104.9 3113.6 3136.1
3141.0 3180.0 3743.6

TS2

-598.1 45.5 57.2 79.5 108.8 117.6 144.0 173.1 259.3
345.4 400.8 475.8 599.0 655.4 749.6 842.9 854.4 929.5
970.6 989.7 1064.5 1117.3 1143.1 1176.0 1186.4 1241.3 1297.4
1320.7 1390.3 1408.7 1413.7 1472.9 1479.8 1484.0 1505.8 1509.8
1567.6 1842.5 3056.3 3066.8 3068.8 3079.2 3111.9 3132.4 3135.2
3141.8 3185.9 3795.6

TS3

-815.7 49.9 96.6 112.7 132.2 161.5 185.0 235.0 341.6
390.9 449.6 476.8 608.1 673.9 733.3 831.3 875.8 930.6
982.9 985.8 1069.6 1100.9 1142.7 1150.7 1197.0 1258.2 1305.9
1334.1 1388.1 1410.8 1414.4 1441.2 1455.7 1469.8 1481.1 1495.1
1503.0 1838.0 3037.4 3052.0 3068.8 3070.6 3108.3 3122.6 3136.8
3150.4 3186.4 3753.5

TS4

-716.5 35.9 59.7 84.4 101.3 107.7 130.8 176.9 329.2
351.5 400.5 478.3 604.8 673.5 745.6 836.8 861.2 919.1
966.9 983.5 1072.2 1111.7 1140.5 1184.0 1223.4 1291.2 1323.2
1331.1 1361.1 1390.2 1416.4 1445.3 1459.6 1472.1 1481.7 1485.8
1498.9 1847.7 3044.0 3068.7 3069.1 3085.9 3092.4 3118.9 3136.5
3163.5 3183.7 3804.7

TS4'

-853.1 37.2 63.0 80.4 84.3 98.1 112.2 178.3 318.2
352.2 396.7 477.8 602.8 697.2 730.4 829.3 850.7 950.1

960.1 980.8 1069.5 1079.9 1141.7 1187.6 1241.3 1275.5 1319.4
1328.3 1348.2 1389.5 1406.6 1428.5 1456.3 1471.5 1476.8 1481.8
1501.2 1850.4 3046.5 3069.1 3077.7 3080.2 3090.6 3119.7 3136.8
3160.2 3184.7 3803.7

（3） $CH_3C(O)C_4H_9$

TS1

-1460.2 25.9 55.5 85.0 96.9 132.3 175.0 244.9 272.9
281.1 318.0 421.0 442.4 481.8 588.2 715.5 737.2 774.4
851.8 888.6 913.2 928.2 992.0 1010.5 1056.0 1091.0 1139.9
1143.9 1208.1 1224.5 1243.8 1293.3 1316.0 1331.2 1376.7 1414.0
1416.7 1433.7 1453.3 1481.2 1490.2 1499.0 1504.3 1513.4 1823.5
3041.9 3047.4 3060.9 3071.2 3073.0 3079.2 3105.0 3115.5 3132.1
3138.9 3180.2 3743.4

TS2

-599.3 44.5 53.4 67.4 87.6 111.3 122.4 126.9 182.2
244.3 300.9 318.9 459.1 476.7 597.9 656.8 736.7 790.8
857.0 904.5 915.6 969.4 1000.2 1051.3 1081.4 1126.7 1148.7
1174.6 1187.4 1233.9 1284.9 1289.4 1324.0 1368.4 1396.7 1412.4
1417.2 1473.0 1480.0 1481.2 1497.5 1504.8 1511.8 1567.4 1842.4
3042.1 3055.7 3062.1 3066.9 3076.5 3080.8 3113.2 3133.0 3135.3
3139.6 3185.8 3795.4

TS3

-774.0 50.2 64.4 102.7 112.9 120.3 146.1 162.0 249.8
298.3 320.7 431.3 461.6 484.2 608.1 681.9 734.2 784.9
844.3 899.8 927.3 983.7 1010.3 1053.3 1103.2 1112.7 1136.1
1169.2 1196.4 1240.3 1289.8 1301.0 1328.1 1371.3 1395.0 1411.9
1418.8 1433.8 1448.2 1469.3 1481.5 1486.2 1504.5 1510.4 1837.8
3034.7 3038.8 3063.6 3068.7 3070.6 3078.3 3101.4 3135.7 3136.6
3144.5 3186.4 3752.1

TS4

-526.7 31.4 54.5 61.2 90.8 97.5 114.1 130.0 135.9
234.5 301.6 320.1 460.1 479.3 603.7 635.0 739.9 796.4
848.1 892.1 910.8 969.6 998.3 1057.8 1090.4 1140.9 1145.2
1191.6 1199.7 1234.1 1287.4 1319.7 1361.9 1377.7 1393.3 1412.6
1418.8 1460.0 1472.4 1481.7 1484.1 1496.5 1500.2 1669.8 1847.4
3043.6 3056.0 3062.2 3068.7 3074.7 3084.8 3109.8 3124.5 3136.4
3143.7 3183.5 3801.1

TS5

-782.5 27.3 52.9 78.4 93.0 106.2 129.6 140.2 164.4
302.7 320.8 328.8 461.8 477.9 604.0 719.6 766.5 799.1
845.6 877.2 913.4 970.3 989.4 1050.2 1094.1 1111.4 1147.7
1174.6 1198.5 1234.5 1291.4 1304.6 1329.1 1350.5 1376.2 1396.0
1416.6 1450.1 1456.6 1471.6 1477.8 1481.6 1485.3 1504.0 1849.0
3034.3 3042.4 3068.5 3070.7 3076.0 3081.7 3095.0 3118.9 3136.2

3161.9 3183.7 3799.5

TS5'

-709.7 32.6 42.8 47.8 82.9 93.1 110.0 129.3 130.4
283.9 315.6 338.3 454.3 476.1 603.5 710.1 724.0 776.8
847.2 891.4 947.1 989.7 1000.1 1048.7 1077.9 1107.7 1148.7
1185.7 1229.1 1245.7 1285.6 1309.2 1328.0 1333.2 1372.4 1392.7
1412.9 1437.8 1456.0 1472.0 1481.6 1484.5 1496.4 1506.9 1849.3
3043.9 3057.7 3068.8 3074.5 3075.9 3090.6 3092.7 3120.5 3136.3
3158.0 3183.8 3806.8

(4) $CH_3C(O)C_5H_{11}$

TS1

-1458.6 24.7 53.1 61.9 78.5 123.1 138.7 155.7 240.9
249.3 266.4 276.7 401.0 423.7 447.1 481.7 594.9 716.0
734.0 750.7 820.3 854.7 904.6 922.3 942.2 998.5 1007.4
1051.3 1079.8 1091.0 1142.9 1147.7 1206.3 1221.2 1237.1 1273.2
1294.6 1330.0 1336.7 1345.2 1399.2 1415.6 1417.9 1433.6 1453.2
1481.1 1488.4 1492.8 1503.9 1505.7 1514.1 1823.4 3033.3 3042.2
3054.0 3059.1 3063.6 3072.5 3073.5 3091.6 3105.0 3117.2 3128.7
3137.3 3180.1 3743.5

TS2

-598.7 42.8 43.5 61.0 74.0 94.5 111.2 133.3 142.8
178.7 225.2 250.4 292.7 406.4 463.6 475.0 604.3 656.7
732.4 758.6 833.1 852.9 922.4 944.9 959.7 1009.2 1043.5
1069.0 1089.7 1130.2 1151.5 1175.5 1186.6 1225.9 1264.9 1273.5
1314.2 1333.4 1339.4 1387.6 1403.2 1413.3 1416.9 1472.8 1479.9
1480.5 1491.4 1501.3 1506.0 1513.3 1569.7 1842.2 3028.4 3053.5
3055.9 3058.9 3064.4 3066.9 3080.3 3092.7 3114.5 3128.2 3135.3
3137.6 3185.7 3795.1

TS3

-773.9 49.1 53.8 67.7 89.0 111.7 130.2 153.2 164.7
234.0 244.5 295.7 393.6 437.5 463.0 482.2 612.1 686.6
735.5 748.1 830.2 854.8 919.3 930.1 966.2 1022.2 1050.8
1082.6 1104.6 1110.5 1144.2 1169.3 1194.4 1230.1 1269.4 1284.5
1318.6 1336.4 1346.3 1387.2 1405.1 1412.4 1416.2 1434.1 1448.3
1469.6 1481.0 1482.0 1498.0 1505.2 1512.2 1837.7 3021.4 3038.5
3056.1 3058.6 3066.6 3068.7 3071.2 3096.4 3103.0 3128.4 3136.6
3137.8 3186.3 3752.0

TS4

-486.9 33.0 51.2 58.4 78.9 94.3 100.2 122.6 131.1
152.7 225.3 254.4 293.0 409.1 463.7 479.4 607.6 627.0
738.4 765.7 836.5 856.1 920.7 931.0 961.3 1007.6 1047.4
1083.1 1096.7 1146.3 1147.1 1188.8 1206.1 1228.5 1275.1 1295.3
1324.7 1333.1 1363.6 1387.0 1400.9 1412.2 1418.8 1460.1 1472.6
1481.1 1481.9 1490.9 1504.7 1509.5 1676.5 1847.6 3043.1 3045.7

3057.3 3059.0 3064.1 3068.8 3081.8 3091.8 3111.3 3127.8 3136.4
3139.7 3183.4 3798.4

TS5

-539.1 27.1 47.8 70.9 78.1 103.3 106.0 128.0 137.1
166.8 224.6 241.9 294.5 402.1 464.6 478.0 610.3 636.6
725.3 777.0 843.6 848.7 926.6 934.6 959.7 1005.3 1050.6
1085.6 1095.3 1142.3 1150.0 1188.5 1219.0 1242.5 1267.6 1302.6
1322.2 1338.7 1340.4 1385.8 1401.0 1411.0 1417.8 1456.7 1471.9
1480.2 1482.1 1494.9 1499.6 1503.3 1585.4 1848.7 3026.5 3042.4
3054.5 3066.8 3068.5 3071.5 3075.7 3085.5 3117.5 3123.0 3136.2
3147.2 3183.8 3794.8

TS6

-769.2 23.9 39.3 58.0 72.3 81.9 99.5 106.6 137.6
153.2 231.0 293.7 328.8 411.9 467.4 476.6 610.5 714.8
727.7 786.7 812.5 845.1 905.3 927.4 956.7 996.1 1047.0
1080.7 1089.2 1128.8 1149.1 1176.6 1190.1 1266.8 1278.1 1307.7
1327.3 1334.3 1352.0 1358.3 1387.9 1406.9 1421.0 1451.6 1456.3
1472.3 1481.7 1484.3 1490.1 1495.6 1509.6 1848.6 3036.2 3042.0
3043.3 3068.0 3069.1 3073.8 3074.4 3087.0 3095.1 3115.9 3136.2
3158.9 3183.5 3805.7

TS6'

-720.7 25.6 33.1 46.9 59.2 60.9 93.0 106.7 130.3
137.8 215.7 289.2 329.2 403.8 459.2 476.3 609.8 721.2
723.3 753.3 823.1 848.7 926.2 953.6 970.7 1008.5 1038.4
1073.5 1085.4 1108.9 1151.5 1184.4 1210.9 1229.6 1264.9 1290.5
1320.7 1329.2 1332.5 1352.0 1386.2 1398.9 1416.1 1448.5 1456.1
1472.0 1481.6 1483.8 1493.0 1498.5 1509.7 1850.1 3036.3 3042.3
3064.6 3068.3 3068.7 3073.8 3074.5 3087.1 3105.1 3119.4 3136.1
3153.9 3183.6 3808.0

（5）$C_2H_5C(O)C_4H_9$

TS1'

-778.0 24.9 42.0 49.1 51.5 77.3 92.3 113.0 126.0
222.8 246.0 289.3 311.3 343.7 465.1 476.1 647.9 703.2
730.4 748.9 813.5 867.9 917.1 923.4 989.1 1015.9 1042.8
1063.4 1092.7 1111.8 1149.7 1156.0 1222.3 1236.5 1277.9 1284.7
1313.4 1323.7 1331.6 1357.9 1384.6 1412.7 1416.2 1421.8 1453.2
1464.3 1481.8 1490.4 1499.2 1504.8 1513.4 1842.0 3042.8 3046.7
3060.1 3064.1 3069.9 3074.4 3078.8 3102.5 3114.5 3115.9 3131.2
3137.6 3184.8 3806.5

TS1

-1149.7 32.8 40.2 81.0 92.6 122.3 133.1 159.8 239.1
247.0 306.5 329.6 350.3 445.7 466.6 478.4 646.2 695.9
739.1 779.0 821.9 885.0 916.7 927.6 951.8 1008.2 1034.9
1056.3 1069.1 1092.9 1141.6 1150.7 1157.4 1227.3 1264.5 1284.5

1313.8 1322.6 1331.8 1365.4 1396.5 1416.5 1422.6 1439.3 1448.8
1456.4 1464.2 1490.5 1499.3 1505.1 1513.5 1832.5 3040.3 3046.7
3050.6 3060.7 3069.9 3073.1 3078.5 3085.0 3112.7 3115.0 3131.8
3138.6 3186.1 3757.2

TS2

-610.2 28.2 41.1 61.4 77.2 87.8 106.3 123.3 138.4
201.6 243.2 246.6 303.9 332.2 471.1 479.0 622.6 669.7
730.3 767.2 810.9 839.1 921.5 924.7 996.6 1029.0 1049.3
1063.5 1092.5 1109.2 1148.1 1156.6 1163.6 1232.0 1276.5 1287.3
1320.6 1331.6 1354.8 1387.6 1415.2 1415.5 1421.9 1459.7 1486.4
1490.4 1493.5 1499.3 1504.7 1513.4 1551.1 1837.3 3042.4 3046.8
3059.5 3069.9 3073.0 3074.5 3079.6 3097.8 3113.0 3130.6 3136.7
3141.6 3163.4 3799.2

TS3

-594.7 33.0 48.4 53.4 68.4 94.1 100.8 130.0 172.2
212.8 242.0 248.1 303.9 331.5 465.6 477.8 621.6 665.5
737.2 769.7 814.7 848.9 920.6 924.6 997.1 1027.5 1039.8
1067.0 1085.7 1122.6 1146.8 1157.0 1177.4 1221.3 1275.6 1280.2
1298.6 1323.9 1360.8 1393.5 1412.8 1416.6 1420.5 1461.9 1480.8
1497.7 1498.0 1504.4 1505.0 1512.1 1569.1 1837.4 3042.2 3054.8
3055.4 3061.8 3077.0 3079.9 3081.8 3090.3 3113.4 3132.8 3139.3
3155.6 3157.1 3795.3

TS4

-780.2 39.2 51.1 74.1 103.4 114.8 137.4 149.0 212.2
247.4 251.7 303.4 338.2 441.9 464.9 486.7 661.0 687.6
705.7 765.9 813.0 842.9 919.6 952.3 1002.8 1033.2 1039.6
1067.6 1108.5 1116.0 1135.4 1154.3 1173.4 1233.4 1280.0 1292.8
1304.2 1329.0 1360.2 1391.6 1409.6 1418.2 1420.4 1430.3 1445.9
1458.9 1485.9 1498.3 1504.6 1505.4 1510.4 1832.7 3034.9 3039.6
3054.6 3063.5 3071.9 3078.2 3080.9 3088.3 3100.3 3135.5 3144.4
3155.0 3161.2 3748.7

TS5

-676.3 8.1 43.9 57.5 84.5 107.0 115.9 127.9 140.2
209.7 227.8 249.2 307.4 337.7 469.7 479.2 613.0 656.1
706.9 775.4 827.3 843.6 921.5 926.8 1005.7 1020.7 1029.6
1069.6 1091.3 1130.2 1136.7 1156.4 1209.8 1239.8 1280.5 1283.8
1326.5 1359.2 1387.8 1410.8 1415.7 1418.6 1422.6 1453.9 1467.4
1485.6 1496.9 1497.5 1500.5 1504.8 1653.4 1842.1 3047.0 3054.0
3058.6 3061.3 3073.2 3079.6 3081.4 3091.6 3106.2 3118.9 3141.5
3154.6 3157.5 3799.5

TS6

-781.6 24.7 41.8 60.5 76.7 96.0 119.2 147.0 177.4
209.1 245.5 305.5 328.9 337.3 467.4 479.9 656.9 705.4
740.2 795.6 814.5 841.8 894.2 930.9 1005.2 1025.4 1030.2
1058.8 1094.3 1118.4 1136.8 1155.6 1185.2 1230.2 1280.2 1287.4

1308.9 1331.8 1350.9 1365.0 1394.5 1416.7 1420.0 1451.1 1454.0
1465.6 1478.2 1485.8 1497.0 1504.2 1505.0 1844.4 3034.2 3043.0
3056.5 3070.7 3076.9 3079.8 3081.6 3090.0 3095.0 3118.8 3153.8
3159.3 3161.7 3799.6

TS6'

-707.3 28.0 36.7 42.9 55.6 82.3 110.2 113.3 122.5
213.4 239.2 291.1 327.1 343.6 466.3 472.3 655.0 703.7
709.8 751.3 816.2 845.5 916.2 977.1 1005.9 1029.2 1034.0
1054.5 1079.8 1115.7 1139.4 1153.8 1224.9 1242.5 1278.9 1285.3
1313.6 1328.5 1333.7 1363.4 1388.9 1413.5 1419.7 1438.4 1452.9
1465.8 1484.8 1496.7 1497.8 1505.2 1507.0 1844.8 3044.6 3057.4
3057.7 3074.5 3076.4 3080.0 3090.0 3090.5 3093.2 3120.6 3154.4
3157.8 3159.0 3806.9

（6）$C_3H_7C(O)C_3H_7$

TS1'

-847.6 25.0 43.6 56.3 83.5 89.5 98.1 106.7 123.8
225.9 249.9 293.1 347.8 358.5 410.1 472.6 686.1 699.7
706.4 752.3 821.1 886.3 898.7 918.2 957.7 1021.8 1039.2
1069.8 1077.7 1100.0 1151.8 1154.4 1230.8 1262.5 1271.9 1313.3
1318.1 1327.8 1335.0 1352.7 1396.2 1414.8 1419.0 1429.9 1451.5
1463.2 1477.3 1495.0 1501.5 1507.0 1511.8 1844.3 3040.6 3049.6
3058.1 3072.4 3077.6 3082.7 3084.6 3090.4 3112.1 3119.6 3134.8
3139.4 3160.0 3803.7

TS1

-780.7 13.5 39.8 57.7 81.9 103.7 113.5 120.6 139.9
231.1 246.9 306.2 331.6 371.8 417.9 473.6 686.1 696.9
724.6 783.6 815.8 874.3 891.7 905.1 945.6 1013.2 1045.9
1067.6 1073.2 1121.7 1151.3 1157.2 1200.5 1256.9 1299.2 1310.3
1329.1 1332.3 1350.0 1370.5 1402.2 1417.8 1421.9 1447.1 1452.7
1466.1 1487.6 1494.6 1495.0 1506.2 1511.8 1841.1 3041.9 3050.6
3057.6 3068.6 3073.6 3082.6 3086.5 3090.3 3111.3 3115.1 3134.1
3137.9 3160.8 3804.2

TS2

-817.9 33.8 53.4 86.7 97.5 127.3 130.3 159.0 231.9
236.2 247.8 305.0 367.4 404.9 455.5 473.0 672.6 696.8
711.1 755.7 829.8 891.8 906.4 917.2 951.9 1030.8 1050.5
1073.6 1087.7 1113.4 1149.3 1155.0 1159.6 1237.5 1272.5 1303.3
1311.4 1328.3 1344.6 1395.0 1413.2 1417.5 1421.1 1440.5 1449.5
1458.0 1495.0 1495.1 1502.4 1506.6 1511.6 1831.3 3036.5 3043.2
3052.0 3058.6 3069.3 3076.8 3082.6 3107.1 3112.8 3122.3 3135.2
3140.4 3149.9 3750.1

TS3

-593.2 28.8 43.0 54.3 86.7 92.9 109.4 120.3 139.0
224.3 246.4 260.3 306.8 363.9 415.1 470.1 627.9 697.7

744.2 756.2 839.4 883.6 897.9 899.3 950.0 1037.5 1053.0
1065.1 1075.0 1134.8 1145.9 1158.4 1180.1 1222.1 1265.7 1288.4
1305.7 1328.8 1338.1 1398.5 1413.9 1416.3 1420.5 1459.1 1484.4
1494.7 1505.7 1506.1 1510.1 1511.7 1574.0 1836.1 3041.5 3056.2
3057.9 3068.3 3074.0 3081.7 3082.5 3111.5 3112.1 3132.6 3134.0
3138.4 3141.4 3795.7

4. Aldehydes

All frequencies are in cm^{-1}.

(1) C_3H_7CHO

TS1

-436.3 20.6 45.1 81.7 120.1 161.5 195.3 245.2 348.5
546.6 659.9 712.1 780.3 874.3 920.6 975.0 1066.3 1130.8
1139.1 1244.4 1276.1 1319.2 1324.3 1400.7 1419.1 1449.3 1495.7
1505.7 1511.5 1874.4 2209.9 3051.1 3060.8 3080.8 3081.2 3113.1
3135.8 3141.4 3791.5

TS2

-675.1 66.4 82.5 87.8 139.5 195.2 209.0 266.7 354.7
581.4 701.4 755.9 825.3 866.3 953.2 970.2 1066.3 1120.4
1138.1 1159.5 1214.1 1288.4 1310.9 1401.8 1414.2 1422.8 1483.9
1505.5 1507.9 1525.2 1849.1 2970.0 3058.3 3067.4 3079.3 3113.1
3133.9 3143.8 3794.4

TS3

-803.9 74.9 135.3 152.6 167.6 213.4 235.6 343.1 419.0
659.4 664.5 711.6 820.9 884.0 956.4 984.2 1053.0 1104.1
1144.3 1160.1 1259.9 1302.9 1319.7 1400.8 1414.6 1421.9 1440.3
1471.8 1494.9 1504.4 1852.8 2966.2 3035.1 3052.9 3066.7 3109.8
3123.9 3151.7 3764.1

TS4

-737.8 44.9 82.2 104.5 131.6 179.0 198.2 330.0 357.6
662.3 691.5 707.1 824.9 862.3 956.5 969.1 1067.0 1110.4
1153.3 1218.6 1285.1 1319.8 1326.2 1359.9 1409.8 1422.4 1441.0
1458.4 1485.6 1491.7 1861.4 2946.3 3043.1 3065.8 3079.6 3093.4
3119.3 3165.2 3804.5

TS4'

-863.3 55.6 66.6 77.1 91.0 179.5 207.0 315.7 352.4
673.1 690.4 705.6 792.7 900.7 950.2 963.7 1070.6 1077.8
1156.0 1242.7 1265.1 1313.8 1326.5 1339.1 1399.6 1416.4 1426.0
1455.3 1476.1 1500.5 1863.7 2947.8 3045.1 3075.0 3077.8 3091.4
3119.1 3161.4 3803.9

(2) C_4H_9CHO

TS1

-427.8 17.4 38.6 72.0 104.4 123.1 137.3 167.4 246.2

295.7 398.3 547.9 661.1 705.8 744.3 842.1 912.5 932.9
961.8 1052.3 1086.9 1137.4 1142.8 1230.9 1262.4 1294.7 1310.6
1331.8 1370.1 1411.1 1417.2 1449.5 1491.3 1499.4 1504.9 1513.6
1874.6 2213.7 3049.8 3051.4 3060.8 3069.5 3077.7 3084.0 3112.8
3132.0 3139.1 3791.6

TS2

-683.6 59.0 73.2 80.2 106.0 124.3 145.9 226.0 249.4
298.7 400.9 579.7 697.0 740.4 787.1 875.9 903.6 928.4
979.4 1055.7 1087.0 1111.1 1144.3 1164.6 1212.8 1268.6 1283.9
1325.5 1368.1 1409.9 1417.9 1422.4 1480.6 1498.6 1505.5 1512.6
1519.7 1848.7 2970.1 3044.1 3054.3 3062.4 3079.3 3083.0 3112.3
3133.6 3140.5 3794.1

TS3

-759.0 59.0 93.8 121.1 137.9 167.6 173.9 251.9 296.2
399.7 411.3 657.8 669.4 707.1 778.4 861.3 912.8 943.8
1000.5 1053.5 1091.6 1114.7 1140.6 1172.5 1241.6 1286.8 1290.9
1324.2 1369.1 1408.9 1418.5 1422.6 1438.6 1461.7 1485.9 1504.8
1510.4 1852.6 2965.7 3034.9 3037.5 3064.1 3067.0 3079.4 3103.0
3136.3 3145.2 3762.2

TS4

-537.4 37.7 66.6 84.6 105.9 125.7 143.7 179.8 236.6
300.0 399.3 633.7 674.0 698.5 791.9 856.3 908.5 929.3
982.4 1059.5 1084.8 1145.4 1157.0 1195.6 1235.7 1277.3 1317.5
1359.4 1379.3 1412.4 1414.0 1422.7 1458.8 1483.8 1496.5 1500.0
1655.1 1861.2 2944.5 3042.3 3056.0 3059.9 3074.6 3079.2 3109.4
3124.9 3144.9 3800.8

TS5

-788.0 39.0 67.7 102.7 133.9 144.3 162.4 186.0 299.0
328.3 404.5 673.3 695.3 737.5 797.7 851.9 906.0 925.7
974.7 1050.3 1092.0 1111.5 1159.3 1188.8 1238.0 1284.3 1302.4
1326.5 1348.6 1376.1 1413.5 1422.2 1446.5 1456.8 1476.9 1484.5
1504.1 1862.6 2945.1 3035.4 3041.0 3067.7 3072.4 3082.8 3095.6
3118.3 3162.6 3799.8

TS5'

-724.2 32.5 45.1 64.0 98.3 113.9 138.0 178.6 303.4
323.5 385.9 670.1 684.6 724.5 752.8 859.4 912.0 970.1
994.3 1047.1 1077.0 1106.7 1163.2 1227.9 1244.3 1278.3 1306.9
1327.8 1329.2 1371.3 1408.0 1422.4 1432.8 1454.9 1482.5 1494.4
1506.2 1863.1 2943.6 3041.9 3058.5 3071.0 3074.2 3091.1 3093.1
3119.1 3158.8 3806.5

(3) $C_5H_{11}CHO$

TS1

-421.9 18.6 36.3 52.7 96.7 108.7 128.5 140.7 171.6
222.3 248.1 364.3 417.6 550.7 661.8 716.0 732.9 786.6

881.7 906.6 934.0 987.2 1045.7 1073.2 1090.1 1140.4 1146.2
1222.8 1251.4 1278.7 1291.3 1328.0 1334.9 1338.1 1393.4 1413.8
1416.5 1449.4 1488.5 1492.5 1503.8 1505.5 1513.9 1874.5 2216.5
3035.7 3051.4 3053.6 3059.2 3065.7 3069.8 3080.9 3091.6 3114.1
3129.0 3137.2 3791.8

TS2

-682.2 43.9 66.5 73.1 96.7 114.1 133.3 149.4 223.2
226.4 249.4 368.2 418.9 582.1 707.5 734.5 763.2 817.0
894.5 915.2 928.3 997.8 1046.2 1076.5 1089.5 1111.8 1148.1
1166.5 1212.1 1251.5 1262.8 1313.0 1332.7 1336.5 1394.1 1412.1
1415.9 1422.8 1480.0 1491.8 1501.3 1505.6 1513.2 1520.8 1848.7
2970.0 3030.4 3052.8 3055.7 3059.1 3067.8 3080.8 3093.1 3113.4
3128.6 3138.0 3793.9

TS3

-756.3 51.2 69.4 90.9 112.4 151.5 166.1 175.7 235.2
246.7 366.5 409.4 414.8 658.1 672.5 717.4 750.2 826.1
893.2 906.8 929.6 1015.8 1051.1 1080.9 1093.4 1114.7 1146.0
1173.8 1231.7 1266.0 1279.6 1316.1 1334.2 1340.5 1396.4 1412.1
1416.6 1422.5 1438.8 1462.2 1481.7 1498.0 1505.9 1512.2 1852.5
2965.4 3022.2 3036.5 3056.4 3059.2 3066.6 3068.3 3096.9 3104.2
3128.9 3138.6 3761.9

TS4

-496.7 41.0 59.2 67.2 106.7 107.4 130.3 151.3 183.4
223.3 254.8 367.4 420.8 623.2 673.2 710.7 763.8 817.8
902.3 909.9 930.1 999.1 1048.3 1082.7 1095.2 1149.8 1159.8
1202.1 1229.0 1266.9 1294.1 1322.8 1330.1 1365.5 1393.9 1411.8
1415.3 1422.7 1458.6 1481.2 1490.7 1504.8 1509.6 1661.6 1861.4
2944.5 3041.7 3045.4 3057.9 3060.2 3061.4 3075.6 3091.9 3110.9
3128.2 3140.4 3797.9

TS5

-544.6 33.8 61.5 81.6 110.6 118.9 133.2 165.4 180.8
223.2 241.0 368.8 415.6 639.9 671.8 709.3 754.4 831.7
902.4 913.2 933.0 995.9 1052.6 1082.1 1095.2 1145.7 1162.3
1222.0 1240.4 1259.8 1301.2 1324.7 1333.0 1344.2 1391.6 1411.3
1415.6 1422.2 1455.6 1480.5 1494.9 1499.8 1503.5 1575.5 1862.4
2944.3 3027.7 3040.8 3054.8 3066.2 3070.3 3071.9 3085.8 3116.8
3123.4 3147.8 3795.1

TS6

-803.8 41.0 50.8 56.3 73.8 119.6 122.7 134.2 181.3
208.5 338.0 371.7 396.5 670.4 701.8 726.9 740.6 798.6
904.4 910.6 937.7 1002.1 1033.5 1063.0 1085.5 1110.3 1165.1
1221.4 1245.9 1281.0 1305.7 1320.6 1330.7 1335.4 1359.1 1394.9
1413.7 1421.8 1434.4 1455.7 1476.7 1490.6 1495.6 1509.8 1863.5
2943.1 3038.6 3040.8 3053.6 3068.7 3071.8 3072.7 3089.0 3098.3
3116.7 3158.0 3805.6

TS6'

-771.2	32.6	53.1	78.8	92.6	110.3	120.5	153.5	180.0
228.2	329.2	368.5	426.3	669.2	708.4	717.5	772.1	797.8
882.4	902.8	931.5	982.8	1048.8	1078.9	1089.2	1131.4	1156.3
1186.7	1261.1	1275.5	1309.2	1324.6	1331.7	1351.5	1358.8	1399.0
1419.2	1423.1	1448.4	1455.3	1483.6	1488.8	1493.7	1509.1	1862.5
2940.8	3036.9	3040.6	3042.8	3067.9	3069.5	3074.8	3087.5	3095.5
3114.5	3159.7	3805.8						

(4) $C_6H_{13}CHO$

TS1

-418.6	18.2	31.8	49.2	70.2	84.0	116.8	131.3	145.0
172.7	192.9	248.4	276.9	386.2	458.2	549.6	662.1	717.6
729.7	755.4	830.1	900.1	914.3	936.7	1006.6	1035.6	1069.1
1080.4	1092.1	1142.1	1149.8	1217.5	1242.6	1266.3	1278.8	1314.0
1316.4	1333.1	1337.8	1369.7	1404.9	1414.0	1417.2	1449.1	1487.8
1488.6	1496.8	1505.2	1506.7	1514.4	1874.6	2217.6	3034.5	3040.3
3051.5	3052.1	3058.9	3061.9	3069.9	3075.0	3081.7	3094.6	3114.6

TS2

-680.1	39.6	50.6	66.1	83.6	95.5	122.2	131.4	149.1
193.1	229.0	246.5	281.3	386.7	459.9	581.4	708.8	731.8
747.7	788.0	853.4	895.5	924.2	940.8	1013.0	1037.1	1070.8
1081.4	1092.0	1114.0	1151.1	1167.5	1210.0	1241.5	1250.4	1295.8
1310.9	1332.0	1335.5	1368.4	1406.0	1413.6	1416.5	1422.4	1480.2
1489.3	1494.0	1505.1	1505.3	1514.1	1520.9	1848.6	2969.6	3030.9
3040.0	3051.2	3054.4	3059.5	3064.3	3075.8	3080.6	3095.4	3113.8
3129.4	3136.9	3793.9						

TS3

-756.9	42.7	58.2	73.6	90.9	134.4	146.3	164.0	171.7
209.1	247.0	277.1	383.4	418.0	458.0	658.9	673.7	718.0
737.1	788.8	850.7	900.6	924.4	938.7	1027.8	1040.5	1070.3
1088.7	1095.8	1114.6	1149.5	1175.4	1224.3	1252.4	1272.2	1301.0
1316.5	1329.7	1337.3	1369.8	1406.1	1414.9	1417.0	1422.1	1438.2
1461.6	1481.0	1492.0	1501.7	1504.7	1514.0	1852.4	2965.1	3023.1
3036.4	3041.7	3051.0	3059.6	3065.8	3067.3	3076.1	3097.1	3104.4
3129.9	3136.7	3762.1						

TS4

-496.7	40.7	54.9	63.0	68.7	82.7	127.8	135.3	162.6
185.7	197.0	247.0	280.1	386.5	459.5	622.8	672.9	712.2
742.1	802.5	841.1	901.7	928.1	941.7	1011.3	1038.1	1077.9
1086.0	1094.5	1153.2	1161.4	1199.3	1225.4	1259.9	1279.6	1303.7
1316.8	1335.1	1357.8	1371.7	1406.3	1413.2	1417.3	1422.3	1458.2
1479.0	1489.1	1497.9	1505.3	1511.9	1660.3	1861.2	2944.3	3031.3
3041.8	3048.1	3060.0	3060.7	3061.4	3073.2	3076.2	3093.4	3111.2
3130.7	3138.3	3797.9						

TS5

-525.4	31.5	56.5	64.5	78.5	86.6	119.5	140.1	158.6
182.3	198.5	252.0	280.0	388.7	462.0	634.4	671.3	710.2
752.1	776.7	852.2	903.3	930.6	947.2	1013.9	1041.4	1070.0
1086.5	1098.5	1151.8	1162.5	1215.0	1232.0	1254.8	1287.4	1305.6
1317.4	1332.7	1351.0	1377.2	1402.2	1413.2	1418.1	1422.5	1455.7
1478.7	1488.5	1502.7	1504.6	1511.3	1588.2	1862.4	2943.7	3028.9
3040.5	3041.1	3060.6	3061.6	3067.7	3071.4	3077.1	3090.2	3116.2
3132.6	3142.3	3794.8						

TS6

-524.0	12.9	40.3	50.4	67.5	87.5	100.4	129.2	139.3
179.3	196.5	234.6	278.1	387.0	458.7	629.6	669.0	710.4
742.4	789.1	839.4	898.4	925.1	939.0	1019.6	1040.1	1075.0
1086.4	1096.7	1156.2	1165.4	1204.0	1228.2	1250.9	1282.4	1307.5
1327.0	1334.3	1362.4	1377.7	1404.8	1412.1	1419.5	1422.6	1454.9
1480.5	1491.8	1496.3	1499.7	1508.8	1629.5	1862.6	2939.4	3029.7
3039.0	3039.9	3055.4	3066.3	3068.2	3070.6	3079.5	3091.2	3114.6
3123.2	3142.5	3800.9						

TS7

-752.6	30.9	46.8	67.7	91.8	99.1	117.9	138.4	156.3
182.8	195.0	281.2	323.3	387.6	461.2	670.0	710.0	725.9
751.4	793.0	842.4	892.3	917.7	939.9	1010.4	1036.5	1068.7
1082.4	1094.4	1129.9	1165.5	1184.9	1228.4	1254.7	1269.3	1305.0
1319.1	1332.0	1336.4	1351.3	1375.0	1408.4	1417.7	1422.1	1453.9
1456.0	1479.7	1489.3	1491.7	1497.0	1510.9	1862.9	2941.0	3033.8
3034.8	3039.8	3043.1	3065.2	3068.8	3071.1	3079.3	3090.4	3100.3
3114.9	3159.4	3803.0						

TS7'

-704.0	26.6	39.9	61.5	68.4	80.1	93.6	131.6	142.3
180.1	201.3	255.5	334.9	390.2	450.4	669.1	705.9	713.1
731.6	762.4	841.0	911.1	932.5	975.2	1015.5	1033.2	1067.6
1081.6	1086.3	1118.2	1166.7	1215.2	1228.3	1254.5	1274.2	1302.9
1316.8	1329.3	1336.6	1338.2	1371.4	1402.0	1416.0	1422.4	1443.5
1455.9	1484.3	1488.4	1496.8	1501.3	1511.6	1863.0	2941.5	3036.0
3040.2	3044.5	3062.7	3065.1	3068.9	3071.3	3083.4	3088.6	3106.0
3115.4	3155.7	3807.1						

References

1. Mendes, J.; Zhou, C.-W.; Curran, H. J., Theoretical Study of the Rate Constants for the Hydrogen Atom Abstraction Reactions of Esters with OH Radicals. *The Journal of Physical Chemistry A* **2014**, *118*, 4889-4899.