Supplemental Materials

Theoretical Kinetic Studies on Intramolecular H-migration reactions of Peroxy Radicals of Diethoxymethane

Contents:

(1) Rate constants of R3 and R4 with different configurations of transition states.

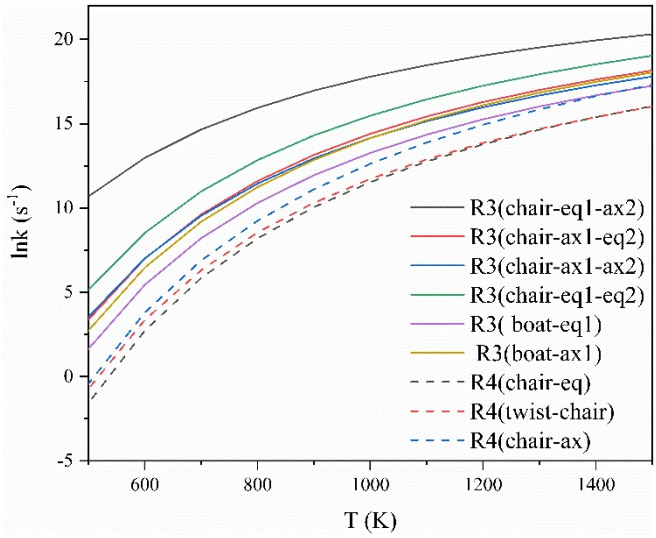

Figure S1. MS-TST/ZCT rate constants of R3 and R4 with different configurations of transition states.

(2) MS-T, MS-LH and SS-HO partition functions of R1, R2, P1, P2, P3 and P4.

Table S1. Conformational-rotational-vibrational partition functions of reactants and products using MS-T and MS-LH, and the harmonic rotational-vibrational partition function (SS-QH) of the lowest energy structure at different temperatures.

T/K	Reactant 1			P1			P2		
	MS-T	MS-LH	SS-HO	MS-T	MS-LH	SS-HO	MS-T	MS-LH	SS-HO
300	1.63E-64	1.00E-64	2.63E-66	1.94E-64	1.10E-64	2.34E-65	1.49E-65	7.33E-65	1.09E-65
400	2.75E-44	1.67E-44	2.96E-46	3.04E-44	1.44E-44	2.09E-45	1.98E-45	9.37E-45	9.30E-46
500	1.22E-31	7.45E-32	9.66E-34	1.48E-31	6.25E-32	6.16E-33	8.96E-33	4.11E-32	2.69E-33
600	8.33E-23	5.15E-23	5.18E-25	1.16E-22	4.57E-23	3.16E-24	6.95E-24	3.11E-23	1.36E-24
700	3.59E-16	2.25E-16	1.84E-18	5.80E-16	2.19E-16	1.10E-17	3.54E-17	1.56E-16	4.75E-18
800	6.27E-11	4.02E-11	2.75E-13	1.16E-10	4.29E-11	1.64E-12	7.36E-12	3.20E-11	7.06E-13
900	1.25E-06	8.19E-07	4.84E-09	2.63E-06	9.61E-07	2.90E-08	1.73E-07	7.44E-07	1.24E-08
1000	5.32E-03	3.56E-03	1.85E-05	1.25E-02	4.56E-03	1.11E-04	8.57E-04	3.65E-03	4.77E-05
1100	7.17E+00	4.92E+00	2.29E-02	1.87E+01	6.83E+00	1.39E-01	1.33E+00	5.63E+00	5.94E-02
1200	4.01E+03	2.82E+03	1.19E+01	1.14E+04	4.21E+03	7.26E+01	8.42E+02	3.55E+03	3.11E+01
1300	1.12E+06	8.10E+05	3.14E+03	3.47E+06	1.29E+06	1.92E+04	2.64E+05	1.11E+06	8.23E+03
1400	1.80E+08	1.33E+08	4.78E+05	5.97E+08	2.24E+08	2.94E+06	4.68E+07	1.97E+08	1.26E+06
1500	1.82E+10	1.38E+10	4.63E+07	6.44E+10	2.45E+10	2.86E+08	5.19E+09	2.19E+10	1.23E+08
T/K	Reactant 2			P3			P4		
	MS-T	MS-LH	SS-HO	MS-T	MS-LH	SS-HO	MS-T	MS-LH	SS-HO
300	1.23E-64	1.63E-64	1.73E-65	1.15E-63	1.33E-63	7.70E-65	7.88E-61	8.44E-61	9.95E-63
400	1.91E-44	2.70E-44	1.87E-45	1.33E-43	1.72E-43	6.13E-45	2.70E-41	3.29E-41	2.33E-43
500	8.10E-32	1.19E-31	5.98E-33	5.08E-31	6.95E-31	1.71E-32	5.04E-29	6.64E-29	3.35E-31
600	5.37E-23	7.99E-23	3.18E-24	3.27E-22	4.58E-22	8.51E-24	2.05E-20	2.80E-20	1.11E-22
700	2.27E-16	3.35E-16	1.12E-17	1.39E-15	1.94E-15	2.92E-17	6.36E-14	8.70E-14	2.89E-16
800	3.91E-11	5.64E-11	1.68E-12	2.45E-10	3.35E-10	4.31E-12	8.92E-09	1.19E-08	3.48E-11
900	7.74E-07	1.08E-06	2.95E-08	4.97E-06	6.57E-06	7.52E-08	1.53E-04	1.97E-04	5.20E-07
1000	3.27E-03	4.35E-03	1.13E-04	2.16E-02	2.74E-02	2.88E-04	5.85E-01	7.12E-01	1.75E-03

1100	4.40E+00	5.56E+00	1.39E-01	2.99E+01	3.60E+01	3.57E-01	7.32E+02	8.35E+02	1.93E+00
1200	2.46E+03	2.94E+03	7.25E+01	1.72E+04	1.95E+04	1.86E+02	3.88E+05	4.13E+05	9.13E+02
1300	6.91E+05	7.74E+05	1.91E+04	4.94E+06	5.29E+06	4.92E+04	1.04E+08	1.03E+08	2.20E+05
1400	1.11E+08	1.17E+08	2.90E+06	8.13E+08	8.16E+08	7.51E+06	1.63E+10	1.48E+10	3.07E+07
1500	1.13E+10	1.11E+10	2.81E+08	8.45E+10	7.95E+10	7.30E+08	1.62E+12	1.36E+12	2.75E+09

(3) The computed thermodynamic properties including enthalpy, heat capacity at constant pressure and entropy of R1, R2, P1, P2, P3 and P4 using MS-T, MS-LH and SS-HO.

Table S2. Enthalpy (kcal·mol-1), heat capacity at constant pressure (cal· mol-1· K-1) and entropy (cal· mol-1· K-1) of R1 using MS-T, MS-LH and SS-HO

	H_T^0			$C_p^0(T)$			S_T^0		
T(K)	SS-HO	MS-LH	MS-T	SS-HO	MS-LH	MS-T	SS-HO	MS-LH	MS-T
300	109.31	110.69	110.72	39.22	42.55	42.34	103.30	113.20	114.28
400	113.53	115.43	115.43	49.09	52.16	51.78	115.94	126.77	127.77
500	118.70	121.09	121.04	58.06	60.75	60.22	127.88	139.36	140.25
600	124.70	127.53	127.43	65.67	68.00	67.32	139.16	151.09	151.88
700	131.40	134.64	134.47	72.03	74.07	73.25	149.77	162.04	162.72
800	138.68	142.31	142.05	77.38	79.18	78.24	159.75	172.28	172.83
900	146.46	150.46	150.09	81.91	83.53	82.48	169.13	181.86	182.30
1000	154.65	159.00	158.53	85.78	87.25	86.11	177.97	190.86	191.18
1100	163.21	167.89	167.30	89.10	90.43	89.23	186.31	199.33	199.54
1200	172.07	177.07	176.36	91.95	93.18	91.92	194.18	207.32	207.42
1300	181.19	186.51	185.67	94.41	95.54	94.25	201.64	214.87	214.87
1400	190.55	196.17	195.20	96.53	97.58	96.28	208.72	222.03	221.93
1500	200.10	206.02	204.92	98.37	99.36	98.05	215.44	228.82	228.64

Table S3. Enthalpy (kcal·mol-1), heat capacity at constant pressure (cal· mol-1· K-1) and entropy (cal· mol-1· K-1) of P1 using MS-T, MS-LH and SS-HO

	H_T^0			$C_p^0(T)$			S_T^0		
T(K)	SS-HO	MS-LH	MS-T	SS-HO	MS-LH	MS-T	SS-HO	MS-LH	MS-T
300	108.68	109.93	110.29	40.46	46.04	48.10	105.59	110.85	113.17
400	113.05	115.10	115.57	50.57	56.86	57.20	118.63	125.65	128.31
500	118.37	121.22	121.68	59.47	65.24	64.72	130.90	139.28	141.90
600	124.51	128.09	128.48	66.88	71.94	71.10	142.42	151.78	154.28
700	131.32	135.57	135.86	73.01	77.40	76.43	153.20	163.30	165.66
800	138.69	143.54	143.73	78.14	81.93	80.90	163.30	173.94	176.16
900	146.54	151.93	152.02	82.50	85.74	84.69	172.76	183.81	185.92
1000	154.78	160.67	160.65	86.22	88.99	87.93	181.65	193.02	195.01
1100	163.37	169.71	169.59	89.42	91.79	90.72	190.02	201.64	203.53
1200	172.26	179.01	178.78	92.18	94.21	93.13	197.92	209.73	211.53
1300	181.41	188.54	188.20	94.56	96.32	95.22	205.39	217.36	219.06
1400	190.77	198.27	197.82	96.64	98.16	97.05	212.48	224.56	226.19
1500	200.34	208.17	207.61	98.44	99.77	98.65	219.21	231.39	232.94

Table S4. Enthalpy (kcal·mol-1), heat capacity at constant pressure (cal· mol-1· K-1) and entropy (cal· mol-1· K-1) of P2 using MS-T, MS-LH and SS-HO

	H_T^0			$C_p^0(T)$			S_T^0		
T(K)	SS-HO	MS-LH	MS-T	SS-HO	MS-LH	MS-T	SS-HO	MS-LH	MS-T
300	108.56	109.86	109.92	40.93	46.04	46.78	103.65	109.81	106.84
400	112.96	115.08	115.19	50.88	58.00	58.38	116.80	124.74	121.94
500	118.31	121.36	121.49	59.68	67.07	67.15	129.13	138.71	135.96
600	124.46	128.40	128.54	67.03	73.51	73.54	140.68	151.54	148.80
700	131.28	136.01	136.16	73.12	78.46	78.51	151.48	163.26	160.52
800	138.66	144.07	144.22	78.22	82.58	82.61	161.59	174.01	171.28
900	146.51	152.51	152.66	82.56	86.13	86.11	171.06	183.95	181.22
1000	154.76	161.28	161.42	86.27	89.24	89.13	179.95	193.19	190.45
1100	163.35	170.34	170.47	89.45	91.97	91.74	188.33	201.83	199.07
1200	172.25	179.66	179.76	92.21	94.37	94.00	196.23	209.93	207.15
1300	181.39	189.21	189.26	94.59	96.47	95.96	203.71	217.57	214.76
1400	190.76	198.95	198.94	96.65	98.31	97.65	210.80	224.79	221.93
1500	200.33	208.86	208.78	98.45	99.92	99.11	217.53	231.63	228.72

Table S5. Enthalpy (kcal·mol-1), heat capacity at constant pressure (cal· mol-1· K-1) and entropy (cal· mol-1· K-1) of R2 using MS-T, MS-LH and SS-HO

	H_T^0			$C_p^0(T)$			S_T^0		
T(K)	SS-HO	MS-LH	MS-T	SS-HO	MS-LH	MS-T	SS-HO	MS-LH	MS-T
300	109.19	110.67	110.51	39.62	43.03	42.87	106.70	113.02	114.10
400	113.45	115.41	115.25	49.37	51.74	51.90	119.44	126.60	127.68
500	118.64	120.99	120.87	58.28	59.51	60.23	131.44	139.09	140.09
600	124.66	127.27	127.26	65.84	66.02	67.37	142.75	150.72	151.53
700	131.37	134.15	134.31	72.17	71.43	73.40	153.39	161.57	162.13
800	138.66	141.53	141.91	77.49	75.98	78.50	163.39	171.72	171.97
900	146.44	149.33	149.98	82.01	79.86	82.84	172.78	181.22	181.15
1000	154.64	157.48	158.46	85.86	83.18	86.57	181.63	190.15	189.74
1100	163.20	165.95	167.28	89.17	86.04	89.77	189.97	198.55	197.80
1200	172.06	174.68	176.40	92.01	88.50	92.53	197.85	206.48	205.40
1300	181.19	183.64	185.77	94.47	90.63	94.92	205.32	213.99	212.57
1400	190.55	192.79	195.37	96.59	92.47	96.99	212.40	221.10	219.35
1500	200.10	202.12	205.16	98.43	94.07	98.78	219.12	227.85	225.79

Table S6. Enthalpy (kcal·mol-1), heat capacity at constant pressure (cal· mol-1· K-1) and entropy (cal· mol-1· K-1) of P3 using MS-T, MS-LH and SS-HO

	H_T^0			$C_p^0(T)$			S_T^0		
T(K)	SS-HO	MS-LH	MS-T	SS-HO	MS-LH	MS-T	SS-HO	MS-LH	MS-T
300	108.38	109.71	109.96	41.46	45.07	45.57	106.91	114.79	115.90
400	112.81	114.70	114.96	51.16	54.53	54.26	120.17	129.07	130.22
500	118.18	120.58	120.77	59.85	62.77	61.79	132.55	142.15	143.17

600	124.34	127.20	127.27	67.13	69.60	68.01	144.12	154.22	155.00
700	131.17	134.46	134.34	73.20	75.26	73.14	154.94	165.39	165.88
800	138.56	142.23	141.87	78.29	80.03	77.44	165.06	175.76	175.94
900	146.42	150.44	149.80	82.61	84.08	81.10	174.54	185.42	185.27
1000	154.67	159.02	158.07	86.32	87.56	84.24	183.44	194.47	193.99
1100	163.27	167.94	166.64	89.50	90.57	86.94	191.82	202.96	202.14
1200	172.17	177.13	175.45	92.25	93.18	89.27	199.73	210.95	209.81
1300	181.32	186.56	184.48	94.62	95.44	91.29	207.20	218.50	217.04
1400	190.69	196.20	193.70	96.69	97.41	93.03	214.29	225.65	223.87
1500	200.26	206.03	203.08	98.49	99.12	94.55	221.03	232.43	230.34

Table S7. Enthalpy (kcal·mol-1), heat capacity at constant pressure (cal· mol-1· K-1) and entropy (cal· mol-1· K-1) of P4 using MS-T, MS-LH and SS-HO

	H_T^0			$C_p^0(T)$			S_T^0		
T(K)	SS-HO	MS-LH	MS-T	SS-HO	MS-LH	MS-T	SS-HO	MS-LH	MS-T
300	107.98	106.76	107.04	41.75	45.76	46.68	104.32	116.57	117.63
400	112.46	111.83	112.16	51.63	55.38	55.37	117.70	131.07	132.28
500	117.88	117.80	118.07	60.34	63.74	62.70	130.18	144.35	145.45
600	124.09	124.53	124.65	67.58	70.63	68.68	141.85	156.60	157.43
700	130.96	131.88	131.77	73.57	76.32	73.61	152.73	167.93	168.39
800	138.38	139.76	139.34	78.60	81.08	77.75	162.89	178.44	178.50
900	146.26	148.07	147.30	82.87	85.11	81.28	172.40	188.23	187.87
1000	154.54	156.76	155.58	86.52	88.56	84.31	181.32	197.38	196.59
1100	163.16	165.77	164.15	89.67	91.53	86.92	189.72	205.97	204.75
1200	172.07	175.05	172.95	92.38	94.09	89.17	197.64	214.04	212.41
1300	181.23	184.58	181.97	94.74	96.30	91.12	205.13	221.66	219.63
1400	190.62	194.30	191.17	96.78	98.21	92.81	212.23	228.87	226.45
1500	200.19	204.21	200.53	98.56	99.88	94.28	218.97	235.70	232.90

(4) Variational transmission coefficients, imaginary frequencies of transition states along with their corresponding crossover temperatures and SCT tunneling transmission coefficients for every pathway of R1-R4.

Table S8. The variational transmission coefficients of every pathway of R1.

T(K)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
300	0.94	0.91	0.99	0.93	0.97	0.95	0.94	0.98	0.82	0.86	0.94	0.79	0.89	0.70	0.74
400	0.93	0.90	0.99	0.91	0.96	0.94	0.93	0.97	0.80	0.84	0.93	0.76	0.87	0.67	0.71
500	0.92	0.89	0.99	0.90	0.96	0.92	0.92	0.97	0.78	0.82	0.92	0.74	0.86	0.66	0.70
600	0.91	0.88	0.99	0.89	0.95	0.91	0.91	0.97	0.76	0.81	0.91	0.72	0.84	0.63	0.68
700	0.90	0.87	0.99	0.88	0.94	0.90	0.90	0.97	0.76	0.80	0.91	0.71	0.83	0.62	0.67
800	0.89	0.86	0.99	0.87	0.94	0.89	0.90	0.97	0.75	0.79	0.90	0.69	0.82	0.60	0.65
900	0.88	0.86	0.99	0.86	0.94	0.89	0.89	0.97	0.74	0.78	0.89	0.68	0.81	0.59	0.64
1000	0.88	0.85	0.99	0.85	0.93	0.88	0.88	0.96	0.73	0.78	0.89	0.67	0.81	0.58	0.63
1100	0.87	0.84	0.99	0.85	0.93	0.87	0.87	0.96	0.72	0.77	0.89	0.66	0.80	0.57	0.62
1200	0.87	0.84	0.99	0.84	0.92	0.87	0.87	0.96	0.71	0.76	0.88	0.65	0.79	0.57	0.62

1300	0.86	0.84	0.99	0.83	0.92	0.86	0.86	0.96	0.70	0.75	0.88	0.64	0.79	0.56	0.61
1400	0.86	0.84	0.99	0.83	0.91	0.85	0.86	0.96	0.70	0.75	0.88	0.64	0.78	0.55	0.60
1500	0.86	0.83	0.99	0.82	0.91	0.85	0.85	0.96	0.69	0.74	0.88	0.63	0.78	0.55	0.60
T(K)	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
300	0.92	0.98	0.99	0.98	0.97	0.99	0.96	0.98	0.95	0.93	0.83	0.94	0.95	0.95	0.92
400	0.90	0.98	0.99	0.98	0.97	0.99	0.96	0.98	0.94	0.92	0.82	0.93	0.95	0.94	0.92
500	0.89	0.98	0.99	0.98	0.96	0.99	0.95	0.98	0.94	0.90	0.81	0.92	0.94	0.94	0.91
600	0.88	0.98	0.99	0.98	0.96	1.00	0.94	0.98	0.93	0.90	0.81	0.91	0.93	0.93	0.91
700	0.87	0.97	0.99	0.98	0.95	0.99	0.94	0.98	0.92	0.89	0.80	0.90	0.93	0.93	0.90
800	0.86	0.97	0.99	0.97	0.95	0.99	0.94	0.98	0.92	0.88	0.80	0.90	0.92	0.93	0.90
900	0.85	0.97	0.99	0.97	0.95	1.00	0.93	0.98	0.91	0.87	0.80	0.89	0.91	0.92	0.90
1000	0.85	0.96	0.99	0.97	0.94	0.99	0.93	0.98	0.91	0.86	0.79	0.89	0.91	0.91	0.89
1100	0.84	0.96	0.99	0.97	0.94	0.99	0.93	0.98	0.90	0.86	0.79	0.88	0.90	0.91	0.89
1200	0.83	0.96	0.99	0.97	0.94	0.99	0.92	0.98	0.89	0.86	0.79	0.88	0.90	0.91	0.89
1300	0.83	0.96	0.99	0.97	0.94	0.99	0.92	0.98	0.89	0.85	0.79	0.87	0.89	0.90	0.89
1400	0.83	0.95	0.99	0.96	0.93	0.99	0.92	0.98	0.88	0.85	0.79	0.87	0.89	0.91	0.89
1500	0.82	0.95	0.99	0.96	0.93	1.00	0.91	0.97	0.88	0.84	0.79	0.86	0.88	0.90	0.89

Table S9. The variational transmission coefficients of every pathway of R2.

T(K)	1	2	3	4
300	0.89	0.75	0.91	0.69
400	0.88	0.73	0.90	0.68
500	0.87	0.71	0.89	0.64
600	0.85	0.70	0.89	0.63
700	0.85	0.69	0.88	0.61
800	0.84	0.68	0.88	0.60
900	0.83	0.67	0.87	0.59
1000	0.82	0.66	0.86	0.58
1100	0.81	0.65	0.86	0.57
1200	0.81	0.65	0.85	0.57
1300	0.80	0.64	0.85	0.56
1400	0.80	0.63	0.84	0.55
1500	0.79	0.63	0.84	0.55

Table S10. The variational transmission coefficients of every pathway of R3.

T(K)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
300	0.84	0.98	0.98	0.98	0.98	0.98	0.99	0.98	0.99	0.98	0.99	0.98	0.99	0.98	0.98
400	0.83	0.97	0.97	0.98	0.98	0.98	0.99	0.97	0.98	0.98	0.98	0.98	0.99	0.98	0.98
500	0.83	0.97	0.97	0.97	0.98	0.98	0.99	0.97	0.98	0.98	0.98	0.98	0.99	0.98	0.98
600	0.82	0.97	0.97	0.97	0.97	0.97	0.99	0.97	0.98	0.98	0.98	0.98	0.98	0.98	0.98
700	0.82	0.97	0.97	0.97	0.97	0.97	0.98	0.97	0.98	0.98	0.98	0.98	0.98	0.98	0.97
800	0.81	0.96	0.96	0.96	0.97	0.97	0.98	0.96	0.98	0.98	0.98	0.98	0.98	0.98	0.97
900	0.81	0.96	0.96	0.96	0.97	0.97	0.98	0.96	0.98	0.97	0.98	0.97	0.98	0.97	0.97
1000	0.80	0.96	0.96	0.96	0.97	0.96	0.98	0.96	0.97	0.97	0.98	0.97	0.98	0.97	0.97
1100	0.80	0.96	0.96	0.95	0.96	0.96	0.98	0.96	0.97	0.97	0.98	0.97	0.98	0.97	0.97
1200	0.80	0.95	0.95	0.95	0.96	0.96	0.98	0.95	0.97	0.97	0.97	0.97	0.98	0.97	0.97

1300	0.80	0.95	0.95	0.95	0.96	0.96	0.98	0.95	0.97	0.97	0.97	0.97	0.97	0.97	0.96
1400	0.79	0.95	0.95	0.94	0.96	0.96	0.98	0.95	0.97	0.97	0.97	0.97	0.97	0.97	0.96
1500	0.79	0.95	0.95	0.94	0.96	0.96	0.98	0.95	0.97	0.97	0.97	0.97	0.97	0.97	0.96
T(K)	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
300	0.97	0.98	0.98	0.99	0.98	0.98	0.98	0.98	0.98	0.98	0.99	0.98	0.98	0.98	0.94
400	0.96	0.98	0.98	0.98	0.98	0.98	0.97	0.98	0.98	0.97	0.99	0.98	0.98	0.98	0.93
500	0.96	0.98	0.97	0.98	0.98	0.98	0.97	0.97	0.98	0.97	0.98	0.98	0.97	0.98	0.92
600	0.95	0.98	0.97	0.98	0.98	0.98	0.97	0.97	0.97	0.97	0.98	0.97	0.97	0.97	0.92
700	0.95	0.98	0.97	0.98	0.98	0.97	0.97	0.97	0.97	0.96	0.98	0.97	0.97	0.97	0.91
800	0.94	0.98	0.96	0.98	0.98	0.97	0.96	0.96	0.97	0.96	0.98	0.97	0.96	0.97	0.90
900	0.94	0.97	0.96	0.98	0.97	0.97	0.96	0.96	0.97	0.96	0.98	0.97	0.96	0.97	0.90
1000	0.94	0.97	0.96	0.98	0.97	0.97	0.96	0.96	0.96	0.96	0.97	0.97	0.96	0.97	0.89
1100	0.93	0.97	0.96	0.97	0.97	0.96	0.96	0.96	0.96	0.95	0.97	0.96	0.96	0.96	0.89
1200	0.93	0.97	0.96	0.97	0.97	0.96	0.95	0.95	0.96	0.95	0.97	0.96	0.95	0.96	0.88
1300	0.93	0.97	0.95	0.97	0.97	0.96	0.95	0.95	0.96	0.95	0.97	0.96	0.95	0.96	0.88
1400	0.93	0.96	0.95	0.97	0.97	0.96	0.95	0.95	0.96	0.95	0.97	0.96	0.95	0.96	0.87
1500	0.92	0.96	0.95	0.97	0.97	0.96	0.95	0.95	0.96	0.94	0.97	0.96	0.95	0.96	0.87
T(K)	31	32	33	34	35	36	37	38	39	40	41	42	43		
300	0.91	0.93	0.90	0.90	0.89	0.87	0.92	0.94	0.92	0.94	0.82	0.84	0.89		
400	0.90	0.91	0.88	0.89	0.88	0.86	0.91	0.94	0.91	0.93	0.81	0.83	0.88		
500	0.89	0.90	0.87	0.88	0.86	0.84	0.90	0.93	0.90	0.92	0.80	0.82	0.86		
600	0.88	0.89	0.86	0.87	0.85	0.83	0.89	0.92	0.89	0.91	0.79	0.81	0.85		
700	0.87	0.88	0.85	0.86	0.84	0.82	0.88	0.92	0.89	0.91	0.79	0.80	0.84		
800	0.86	0.87	0.84	0.85	0.83	0.81	0.87	0.91	0.88	0.90	0.76	0.79	0.83		
900	0.85	0.87	0.83	0.85	0.82	0.81	0.87	0.91	0.87	0.89	0.75	0.77	0.82		
1000	0.84	0.86	0.82	0.84	0.81	0.80	0.86	0.90	0.87	0.89	0.74	0.77	0.81		
1100	0.84	0.85	0.81	0.83	0.80	0.79	0.85	0.90	0.86	0.88	0.74	0.76	0.80		
1200	0.83	0.84	0.81	0.82	0.80	0.78	0.84	0.90	0.86	0.88	0.73	0.75	0.80		
1300	0.83	0.84	0.80	0.82	0.79	0.78	0.84	0.89	0.85	0.87	0.73	0.75	0.79		
1400	0.82	0.83	0.80	0.81	0.78	0.77	0.83	0.89	0.85	0.87	0.72	0.74	0.78		
1500	0.82	0.83	0.79	0.81	0.78	0.77	0.83	0.89	0.84	0.86	0.72	0.74	0.78		

Table S11. The variational transmission coefficients of every pathway of R4.

T(K)	1	2	3	4	5	6	7	8
300	0.96	0.96	0.95	0.96	0.96	0.94	0.96	0.96
400	0.95	0.95	0.95	0.95	0.95	0.94	0.95	0.95
500	0.95	0.95	0.95	0.95	0.95	0.93	0.94	0.95
600	0.94	0.95	0.94	0.94	0.94	0.93	0.94	0.94
700	0.94	0.94	0.94	0.94	0.94	0.92	0.93	0.94
800	0.94	0.94	0.93	0.93	0.94	0.92	0.93	0.93
900	0.93	0.94	0.93	0.93	0.93	0.91	0.92	0.93
1000	0.93	0.94	0.93	0.93	0.93	0.91	0.92	0.92
1100	0.93	0.93	0.93	0.92	0.93	0.90	0.92	0.92
1200	0.92	0.93	0.92	0.92	0.92	0.90	0.91	0.92
1300	0.92	0.93	0.92	0.92	0.92	0.90	0.91	0.92

1400	0.92	0.93	0.92	0.92	0.92	0.89	0.91	0.91
1500	0.92	0.93	0.92	0.91	0.92	0.89	0.90	0.91
T(K)	9	10	11	12	13	14	15	16
300	0.96	0.95	0.95	0.97	0.97	0.96	0.95	0.96
400	0.95	0.95	0.94	0.96	0.97	0.95	0.95	0.95
500	0.94	0.94	0.93	0.96	0.96	0.95	0.94	0.94
600	0.94	0.94	0.93	0.95	0.96	0.94	0.94	0.94
700	0.93	0.94	0.92	0.95	0.96	0.94	0.93	0.93
800	0.93	0.93	0.92	0.94	0.95	0.94	0.93	0.93
900	0.93	0.93	0.92	0.94	0.95	0.93	0.92	0.92
1000	0.92	0.92	0.91	0.94	0.95	0.93	0.92	0.92
1100	0.92	0.92	0.91	0.93	0.94	0.93	0.92	0.92
1200	0.92	0.92	0.90	0.93	0.94	0.93	0.91	0.91
1300	0.91	0.92	0.90	0.93	0.94	0.92	0.91	0.91
1400	0.91	0.91	0.90	0.92	0.93	0.92	0.91	0.91
1500	0.91	0.91	0.90	0.92	0.93	0.92	0.90	0.90
T(K)	17	18	19	20	21	22	23	
300	0.95	0.94	0.95	0.95	0.95	0.96	0.96	
400	0.94	0.93	0.94	0.95	0.94	0.95	0.95	
500	0.93	0.92	0.94	0.94	0.94	0.94	0.94	
600	0.93	0.91	0.93	0.94	0.93	0.94	0.94	
700	0.92	0.91	0.92	0.93	0.93	0.94	0.94	
800	0.92	0.90	0.92	0.93	0.92	0.93	0.93	
900	0.91	0.89	0.91	0.92	0.92	0.93	0.93	
1000	0.91	0.89	0.91	0.92	0.92	0.92	0.92	
1100	0.90	0.88	0.90	0.92	0.91	0.92	0.92	
1200	0.90	0.88	0.90	0.91	0.91	0.92	0.92	
1300	0.89	0.87	0.89	0.91	0.91	0.91	0.91	
1400	0.89	0.87	0.89	0.91	0.91	0.91	0.91	
1500	0.89	0.86	0.89	0.90	0.90	0.91	0.91	

Table S12. The magnitudes of imaginary frequencies (fre) of transition states along with their corresponding crossover temperatures (T_c) and SCT tunneling transmission coefficients for every pathway of R1.

	1	2	3	4	5	6	7	8	9	10
fre(cm^{-1})	1734.43	1709.28	1895.42	1714.99	1679.29	1699.37	1686.51	1861.34	1710.2	1709.76
T_c(K)	397.66	391.89	434.57	393.20	385.01	389.62	386.67	426.75	392.10	392.00
300	54.42	30.87	114.43	68.47	31.35	51.71	27.15	111.60	377.57	41.54
400	8.38	6.75	11.25	7.96	6.69	7.43	6.32	11.24	8.60	6.86
500	3.80	3.37	4.52	3.62	3.33	3.51	3.25	4.53	3.56	3.41
600	2.50	2.32	2.81	2.41	2.29	2.37	2.26	2.81	2.36	2.34
700	1.95	1.85	2.12	1.89	1.83	1.88	1.82	2.11	1.86	1.87
800	1.66	1.60	1.77	1.62	1.59	1.62	1.58	1.77	1.60	1.61
900	1.49	1.45	1.57	1.46	1.44	1.46	1.43	1.56	1.45	1.46

1000	1.38	1.35	1.44	1.36	1.34	1.36	1.34	1.43	1.35	1.36
1100	1.30	1.28	1.35	1.29	1.27	1.29	1.27	1.34	1.28	1.29
1200	1.25	1.23	1.28	1.24	1.23	1.24	1.22	1.28	1.23	1.24
1300	1.21	1.19	1.24	1.20	1.19	1.20	1.19	1.23	1.19	1.20
1400	1.18	1.16	1.20	1.17	1.16	1.17	1.16	1.20	1.16	1.17
1500	1.15	1.14	1.17	1.15	1.14	1.14	1.14	1.17	1.14	1.15
	11	12	13	14	15	16	17	18	19	20
fre(cm^{-1})	1939.57	1678.35	1690.92	1666.34	1687.98	1883.02	1805.86	1855.28	1814	1792.29
T_c(K)	444.69	384.80	387.68	382.05	387.01	431.72	414.03	425.36	415.90	410.92
300	930.60	706.49	80.59	466.18	96.33	677.94	68.24	100.29	77.57	76.32
400	15.02	7.89	7.29	7.29	6.88	12.29	10.37	10.26	10.39	10.75
500	5.03	3.28	3.35	3.16	3.24	4.46	4.36	4.27	4.32	4.43
600	2.96	2.23	2.27	2.18	2.23	2.72	2.74	2.71	2.72	2.76
700	2.18	1.79	1.81	1.76	1.79	2.05	2.08	2.07	2.07	2.09
800	1.80	1.55	1.57	1.54	1.56	1.72	1.74	1.75	1.73	1.75
900	1.58	1.41	1.43	1.40	1.42	1.53	1.55	1.55	1.54	1.55
1000	1.45	1.32	1.33	1.31	1.32	1.41	1.42	1.43	1.42	1.42
1100	1.36	1.26	1.27	1.25	1.26	1.32	1.34	1.34	1.33	1.34
1200	1.29	1.21	1.22	1.21	1.21	1.26	1.27	1.28	1.27	1.28
1300	1.24	1.18	1.18	1.17	1.18	1.22	1.23	1.23	1.23	1.23
1400	1.20	1.15	1.16	1.15	1.15	1.19	1.19	1.20	1.19	1.20
1500	1.18	1.13	1.13	1.13	1.13	1.16	1.17	1.17	1.17	1.17
	21	22	23	24	25	26	27	28	29	30
fre(cm^{-1})	1877.16	1750.07	1867.57	1732.73	1800.06	1909.84	1795.69	1682.05	1831.31	1929.92
T_c(K)	430.38	401.24	428.18	397.27	412.70	437.87	411.70	385.65	419.87	442.48
300	109.46	52.50	78.88	46.82	70.48	304.14	94.95	32.02	133.65	495.63
400	10.78	9.05	9.72	8.13	9.22	11.64	10.20	6.62	11.08	13.44
500	4.39	4.09	4.17	3.76	3.98	4.43	4.18	3.34	4.38	4.87
600	2.75	2.65	2.67	2.49	2.56	2.75	2.63	2.31	2.72	2.94
700	2.09	2.04	2.05	1.94	1.98	2.08	2.01	1.85	2.06	2.18
800	1.75	1.72	1.73	1.66	1.68	1.74	1.70	1.60	1.73	1.81
900	1.55	1.54	1.54	1.49	1.50	1.54	1.51	1.45	1.53	1.59
1000	1.43	1.41	1.42	1.38	1.39	1.42	1.39	1.35	1.41	1.45
1100	1.34	1.33	1.33	1.30	1.31	1.33	1.31	1.28	1.33	1.36
1200	1.28	1.27	1.27	1.25	1.25	1.27	1.26	1.23	1.27	1.29
1300	1.23	1.23	1.23	1.21	1.21	1.23	1.21	1.19	1.22	1.25
1400	1.20	1.19	1.19	1.18	1.18	1.19	1.18	1.17	1.19	1.21
1500	1.17	1.17	1.17	1.15	1.15	1.17	1.16	1.14	1.16	1.18

Table S13. The magnitudes of imaginary frequencies (fre) of transition states along with their corresponding crossover temperatures (T_c) and SCT tunneling transmission coefficients for every pathway of R2.

	1	2	3	4
fre(cm^{-1})	1778.36	1776.38	1804.94	1823.20
T_c(K)	407.73	407.27	413.82	418.01

300	45.79	47.30	53.39	54.97
400	8.76	9.26	10.14	10.42
500	4.06	4.28	4.53	4.72
600	2.66	2.77	2.88	3.00
700	2.06	2.13	2.18	2.27
800	1.74	1.79	1.82	1.88
900	1.55	1.58	1.61	1.65
1000	1.43	1.45	1.47	1.50
1100	1.34	1.36	1.37	1.40
1200	1.28	1.30	1.31	1.33
1300	1.24	1.25	1.26	1.28
1400	1.20	1.21	1.22	1.23
1500	1.17	1.18	1.19	1.20

Table S14. The magnitudes of imaginary frequencies (fre) of transition states along with their corresponding crossover temperatures (T_c) and SCT tunneling transmission coefficients for every pathway of R3.

	1	2	3	4	5	6	7	8	9	10
fre(cm^{-1})	1790.867	1784.1758	1787.01	1744.114	1760.323	1739.68	1786.655	1806.004	1803.132	1790.246
T_c(K)	410.60	409.06	409.71	399.88	403.59	398.86	409.63	414.07	413.41	410.45
300	53.37	46.72	53.19	43.17	46.55	46.27	47.01	46.72	60.23	50.74
400	8.53	8.40	8.77	8.19	8.80	8.69	8.02	8.40	8.77	8.41
500	3.89	3.87	3.96	3.79	3.99	3.95	3.77	3.87	4.00	3.91
600	2.55	2.55	2.59	2.50	2.60	2.57	2.52	2.55	2.62	2.58
700	1.98	1.98	2.00	1.95	2.01	1.99	1.97	1.98	2.03	2.01
800	1.68	1.68	1.70	1.66	1.70	1.69	1.68	1.68	1.72	1.71
900	1.51	1.51	1.52	1.49	1.52	1.51	1.51	1.51	1.53	1.53
1000	1.39	1.39	1.40	1.38	1.40	1.39	1.40	1.39	1.41	1.41
1100	1.31	1.31	1.32	1.31	1.32	1.31	1.32	1.31	1.33	1.33
1200	1.26	1.26	1.26	1.25	1.26	1.26	1.26	1.26	1.27	1.27
1300	1.22	1.22	1.22	1.21	1.22	1.22	1.22	1.22	1.23	1.23
1400	1.18	1.18	1.19	1.18	1.19	1.18	1.19	1.18	1.19	1.19
1500	1.16	1.16	1.16	1.15	1.16	1.16	1.16	1.16	1.17	1.16
	11	12	13	14	15	16	17	18	19	20
fre(cm^{-1})	1808.3392	1812.714	1780.452	1809.519	1787.88	1770.536	1767.776	1742.919	1752.376	1745.119
T_c(K)	414.60	415.61	408.21	414.87	409.91	405.93	405.30	399.60	401.77	400.11
300	63.51	70.19	47.59	60.65	84.69	54.29	53.48	40.60	44.01	44.08
400	8.74	8.77	8.21	8.44	9.20	8.23	8.99	8.07	8.64	8.49
500	3.95	3.97	3.85	3.87	4.05	3.80	4.12	3.84	4.04	3.98
600	2.59	2.61	2.56	2.56	2.63	2.52	2.69	2.56	2.65	2.62
700	2.01	2.02	2.00	1.99	2.03	1.97	2.07	2.00	2.05	2.03
800	1.71	1.71	1.70	1.69	1.72	1.68	1.75	1.70	1.74	1.72
900	1.52	1.53	1.52	1.52	1.53	1.50	1.56	1.52	1.55	1.54
1000	1.41	1.41	1.40	1.40	1.41	1.39	1.43	1.40	1.42	1.42
1100	1.33	1.33	1.32	1.32	1.33	1.31	1.35	1.32	1.34	1.33

1200	1.27	1.27	1.27	1.26	1.27	1.26	1.28	1.27	1.28	1.27
1300	1.22	1.23	1.22	1.22	1.23	1.21	1.24	1.22	1.23	1.23
1400	1.19	1.19	1.19	1.19	1.19	1.18	1.20	1.19	1.20	1.19
1500	1.16	1.17	1.16	1.16	1.17	1.16	1.17	1.16	1.17	1.17
	21	22	23	24	25	26	27	28	29	30
fre(cm^{-1})	1808.3455	1805.5755	1802.382	1826.416	1819.503	1824.167	1821.03	1831.351	1803.516	1877.664
T_c(K)	414.60	413.97	413.24	418.75	417.16	418.23	417.51	419.88	413.50	430.50
300	39.05	43.92	42.80	55.25	49.68	79.80	60.30	80.30	75.42	197.07
400	7.52	8.10	7.96	8.96	8.27	9.55	9.09	9.53	9.13	13.04
500	3.59	3.80	3.74	4.03	3.82	4.08	4.03	4.11	4.00	4.76
600	2.42	2.52	2.49	2.62	2.53	2.61	2.61	2.64	2.59	2.85
700	1.91	1.97	1.95	2.02	1.97	2.01	2.01	2.03	2.00	2.12
800	1.64	1.68	1.66	1.71	1.68	1.70	1.70	1.71	1.69	1.76
900	1.47	1.51	1.49	1.53	1.50	1.51	1.52	1.53	1.51	1.56
1000	1.37	1.39	1.38	1.41	1.39	1.40	1.40	1.41	1.40	1.43
1100	1.30	1.31	1.31	1.33	1.31	1.32	1.32	1.33	1.32	1.34
1200	1.24	1.26	1.25	1.27	1.26	1.26	1.26	1.27	1.26	1.28
1300	1.20	1.22	1.21	1.22	1.21	1.22	1.22	1.22	1.22	1.23
1400	1.17	1.18	1.18	1.19	1.18	1.18	1.19	1.19	1.18	1.20
1500	1.15	1.16	1.15	1.16	1.16	1.16	1.16	1.16	1.16	1.17
T(K)	31	32	33	34	35	36	37	38	39	40
fre(cm^{-1})	1875.2638	1874.0158	1872.057	1878.458	1876.715	1847.606	1865.308	1848.875	1853.208	1851.243
T_c(K)	429.95	429.66	429.21	430.68	430.28	423.61	427.66	423.90	424.89	424.44
300	160.29	151.59	188.76	168.51	230.40	118.46	80.78	112.84	94.35	126.13
400	12.82	12.13	12.59	13.85	12.98	10.92	10.29	10.77	10.67	11.66
500	4.70	4.58	4.60	4.98	4.66	4.35	4.23	4.36	4.36	4.60
600	2.82	2.78	2.78	2.94	2.79	2.71	2.65	2.72	2.72	2.83
700	2.10	2.09	2.08	2.17	2.09	2.05	2.02	2.06	2.07	2.12
800	1.75	1.74	1.74	1.79	1.74	1.72	1.70	1.73	1.73	1.77
900	1.55	1.54	1.54	1.58	1.54	1.53	1.52	1.54	1.54	1.56
1000	1.42	1.42	1.41	1.44	1.41	1.41	1.40	1.41	1.42	1.43
1100	1.33	1.33	1.33	1.35	1.33	1.33	1.32	1.33	1.33	1.34
1200	1.27	1.27	1.27	1.29	1.27	1.27	1.26	1.27	1.27	1.28
1300	1.23	1.23	1.22	1.24	1.22	1.22	1.22	1.22	1.23	1.23
1400	1.19	1.19	1.19	1.20	1.19	1.19	1.18	1.19	1.19	1.20
1500	1.17	1.16	1.16	1.17	1.16	1.16	1.16	1.16	1.16	1.17
T(K)	41	42	43							
fre(cm^{-1})	1840.2793	1852.2051	1827.241							
T_c(K)	421.93	424.66	418.94							
300	109.70	118.99	230.40							
400	10.36	11.69	12.98							
500	4.22	4.58	4.66							
600	2.65	2.81	2.79							
700	2.03	2.11	2.09							

800	1.71	1.76	1.74
900	1.52	1.56	1.54
1000	1.40	1.43	1.41
1100	1.32	1.34	1.33
1200	1.26	1.28	1.27
1300	1.22	1.23	1.22
1400	1.19	1.20	1.19
1500	1.16	1.17	1.16

Table S15. The magnitudes of imaginary frequencies (fre) of transition states along with their corresponding crossover temperatures (T_c) and SCT tunneling transmission coefficients for every pathway of R4.

	1	2	3	4	5	6	7	8	9	10
fre(cm^{-1})	1900.21	1907.13	1903.32	1904.13	1901.67	1897.27	1907.37	1910.51	1911.09	1906.56
T_c(K)	435.67	437.25	436.38	436.56	436.00	434.99	437.31	438.03	438.16	437.12
300	86.86	79.50	84.82	117.28	115.76	105.72	99.48	112.17	103.27	73.22
400	11.21	11.34	10.76	11.63	12.54	10.48	11.72	13.22	11.35	10.26
500	4.79	4.86	4.64	4.81	5.10	4.47	4.89	5.31	4.71	4.44
600	3.03	3.06	2.96	3.02	3.16	2.86	3.06	3.24	2.96	2.83
700	2.28	2.31	2.25	2.28	2.35	2.18	2.29	2.40	2.23	2.16
800	1.90	1.91	1.87	1.89	1.94	1.82	1.90	1.97	1.86	1.81
900	1.67	1.68	1.65	1.66	1.69	1.61	1.67	1.71	1.63	1.60
1000	1.52	1.52	1.50	1.51	1.54	1.48	1.52	1.55	1.49	1.46
1100	1.41	1.42	1.40	1.41	1.43	1.38	1.41	1.44	1.39	1.37
1200	1.34	1.34	1.33	1.34	1.35	1.31	1.34	1.36	1.32	1.30
1300	1.28	1.29	1.28	1.28	1.29	1.26	1.28	1.30	1.27	1.25
1400	1.24	1.24	1.23	1.24	1.25	1.22	1.24	1.25	1.23	1.22
1500	1.21	1.21	1.20	1.20	1.21	1.19	1.21	1.22	1.20	1.19
T(K)	11	12	13	14	15	16	17	18	19	20
fre(cm^{-1})	1899.50	1908.49	1841.64	1868.88	1922.30	1914.63	1879.71	1879.13	1873.10	1881.59
T_c(K)	435.50	437.56	422.24	428.48	440.73	438.97	430.97	430.83	429.45	431.40
300	88.57	85.22	84.40	75.50	63.42	68.07	79.69	75.84	84.83	103.68
400	12.52	11.55	9.88	10.48	10.50	10.58	12.87	11.53	12.68	12.62
500	5.17	4.86	4.32	4.59	4.59	4.57	5.33	4.88	5.21	5.14
600	3.18	3.04	2.79	2.93	2.91	2.89	3.25	3.04	3.18	3.16
700	2.36	2.28	2.14	2.23	2.21	2.19	2.40	2.28	2.35	2.35
800	1.94	1.89	1.80	1.86	1.84	1.83	1.96	1.88	1.93	1.93
900	1.69	1.66	1.60	1.64	1.62	1.61	1.71	1.65	1.68	1.69
1000	1.54	1.51	1.46	1.50	1.48	1.47	1.54	1.50	1.53	1.53
1100	1.43	1.41	1.37	1.40	1.38	1.38	1.43	1.40	1.42	1.42
1200	1.35	1.33	1.31	1.33	1.31	1.31	1.35	1.33	1.34	1.35
1300	1.29	1.28	1.26	1.27	1.26	1.26	1.29	1.27	1.29	1.29
1400	1.25	1.24	1.22	1.23	1.22	1.22	1.25	1.23	1.24	1.25
1500	1.21	1.20	1.19	1.20	1.19	1.19	1.21	1.20	1.21	1.21
T(K)	21	22	23							

fre(cm^{-1})	1882.77	1889.82	1879.63
T_c(K)	431.67	433.28	430.95
300	129.92	117.40	117.40
400	13.57	12.85	12.85
500	5.40	5.21	5.21
600	3.29	3.20	3.20
700	2.42	2.37	2.37
800	1.98	1.95	1.95
900	1.72	1.70	1.70
1000	1.56	1.54	1.54
1100	1.45	1.43	1.43
1200	1.36	1.35	1.35
1300	1.30	1.29	1.29
1400	1.26	1.25	1.25
1500	1.22	1.21	1.21

(5) Multi-structure torsional anharmonicity factors and generalized transmission coefficients for R1-R4.

Table S16. Multi-structure torsional anharmonicity factors (F_{act}) and generalized transmission coefficients (γ) for R1 and R2.

T/K	R1		R2	
	Multi-structure torsional anharmonicity factors	Generalized transmission coefficients	Multi-structure torsional anharmonicity factors	Generalized transmission coefficients
300	0.1038	54.0226	0.0225	39.8830
400	0.0934	7.7354	0.0184	7.5029
500	0.0883	3.4671	0.0158	3.3643
600	0.0864	2.2586	0.0141	2.1344
700	0.0863	1.7451	0.0128	1.6015
800	0.0874	1.4760	0.0120	1.3192
900	0.0891	1.3138	0.0114	1.1474
1000	0.0914	1.2071	0.0109	1.0341
1100	0.0939	1.1322	0.0105	0.9543
1200	0.0967	1.0784	0.0103	0.8966
1300	0.0996	1.0371	0.0101	0.8511
1400	0.1025	1.0047	0.0100	0.8158
1500	0.1056	0.9790	0.0099	0.7871
	R3		R4	
T/K	Multi-structure torsional anharmonicity factors	Generalized transmission coefficients	Multi-structure torsional anharmonicity factors	Generalized transmission coefficients
300	0.6334	44.8390	0.7838	73.5949
400	0.6660	8.3174	0.7395	11.0816
500	0.7206	3.8084	0.7156	4.6401

600	0.7811	2.4906	0.7039	2.8751
700	0.8394	1.9266	0.7006	2.1422
800	0.8913	1.6292	0.7034	1.7631
900	0.9352	1.4506	0.7103	1.5392
1000	0.9708	1.3336	0.7201	1.3945
1100	0.9985	1.2521	0.7318	1.2940
1200	1.0189	1.1927	0.7446	1.2221
1300	1.0330	1.1477	0.7578	1.1683
1400	1.0416	1.1126	0.7712	1.1260
1500	1.0456	1.0845	0.7843	1.0927

(6) High-pressure limit rate constants of every pathway of R1-R4 calculated by using TST.

Table S17. Rate constants for R1 with chair-eq transition states.

	chair-eq							
T (K)	1	2	3	4	5	6	7	8
300	1.93E-04	2.65E-02	3.35E-05	1.82E-05	1.32E-03	4.41E-05	2.23E-03	2.55E-06
400	2.81E+00	1.17E+02	7.75E-01	4.68E-01	7.17E+00	8.21E-01	1.38E+01	1.02E-01
500	9.13E+02	1.86E+04	3.35E+02	2.15E+02	1.29E+03	3.10E+02	2.68E+03	6.12E+01
600	4.43E+04	5.60E+05	1.97E+04	1.32E+04	4.23E+04	1.66E+04	9.26E+04	4.49E+03
700	7.23E+05	6.52E+06	3.70E+05	2.53E+05	5.20E+05	2.90E+05	1.19E+06	9.84E+04
800	5.95E+06	4.18E+07	3.39E+06	2.36E+06	3.47E+06	2.52E+06	8.16E+06	1.01E+06
900	3.10E+07	1.79E+08	1.92E+07	1.36E+07	1.54E+07	1.37E+07	3.69E+07	6.29E+06
1000	1.17E+08	5.78E+08	7.75E+07	5.53E+07	5.09E+07	5.35E+07	1.25E+08	2.73E+07
1100	3.50E+08	1.52E+09	2.45E+08	1.76E+08	1.36E+08	1.64E+08	3.40E+08	9.16E+07
1200	8.74E+08	3.41E+09	6.41E+08	4.64E+08	3.12E+08	4.19E+08	7.88E+08	2.52E+08
1300	1.90E+09	6.80E+09	1.45E+09	1.06E+09	6.29E+08	9.32E+08	1.61E+09	5.97E+08
1400	3.73E+09	1.23E+10	2.95E+09	2.15E+09	1.15E+09	1.85E+09	2.98E+09	1.25E+09
1500	6.68E+09	2.06E+10	5.44E+09	3.99E+09	1.95E+09	3.37E+09	5.09E+09	2.39E+09

Table S18. Rate constants for R1 with boat-eq transition states.

	boat-eq							
T (K)	9	10	11	12	13	14	15	16
300	6.58E-08	6.03E-07	1.19E-08	7.56E-09	2.55E-07	2.27E-08	3.57E-07	9.93E-10
400	7.20E-03	2.91E-02	1.99E-03	1.39E-03	1.27E-02	3.13E-03	2.10E-02	2.75E-04
500	7.88E+00	1.95E+01	2.80E+00	2.08E+00	8.68E+00	3.92E+00	1.59E+01	5.26E-01
600	8.58E+02	1.54E+03	3.63E+02	2.80E+02	6.89E+02	4.69E+02	1.35E+03	8.33E+01
700	2.49E+04	3.56E+04	1.20E+04	9.46E+03	1.60E+04	1.46E+04	3.31E+04	3.17E+03
800	3.16E+05	3.82E+05	1.68E+05	1.35E+05	1.72E+05	1.94E+05	3.69E+05	4.95E+04
900	2.31E+06	2.45E+06	1.32E+06	1.07E+06	1.10E+06	1.47E+06	2.44E+06	4.24E+05
1000	1.14E+07	1.09E+07	6.95E+06	5.70E+06	4.91E+06	7.52E+06	1.11E+07	2.38E+06
1100	4.25E+07	3.73E+07	2.72E+07	2.25E+07	1.68E+07	2.87E+07	3.89E+07	9.86E+06
1200	1.28E+08	1.04E+08	8.53E+07	7.09E+07	4.69E+07	8.82E+07	1.11E+08	3.24E+07
1300	3.25E+08	2.50E+08	2.25E+08	1.88E+08	1.13E+08	2.29E+08	2.69E+08	8.88E+07
1400	7.27E+08	5.32E+08	5.20E+08	4.35E+08	2.39E+08	5.19E+08	5.79E+08	2.12E+08

1500	1.46E+09	1.02E+09	1.08E+09	9.03E+08	4.60E+08	1.06E+09	1.13E+09	4.51E+08

Table S19. Rate constants for R1 with chair-ax transition states.

	chair-ax							
T (K)	17	18	19	20	21	22	23	24
300	2.39E-03	2.32E-04	1.15E-04	4.03E-04	1.10E-05	4.97E-06	4.18E-05	1.13E-05
400	1.54E+01	2.94E+00	1.43E+00	3.71E+00	2.77E-01	1.07E-01	7.28E-01	1.99E-01
500	3.06E+03	8.84E+02	4.21E+02	9.15E+02	1.25E+02	4.42E+01	2.64E+02	7.29E+01
600	1.07E+05	4.09E+04	1.92E+04	3.69E+04	7.60E+03	2.52E+03	1.38E+04	3.84E+03
700	1.38E+06	6.45E+05	2.99E+05	5.28E+05	1.46E+05	4.63E+04	2.39E+05	6.65E+04
800	9.57E+06	5.20E+06	2.38E+06	3.94E+06	1.36E+06	4.16E+05	2.06E+06	5.74E+05
900	4.35E+07	2.67E+07	1.21E+07	1.90E+07	7.80E+06	2.33E+06	1.11E+07	3.10E+06
1000	1.47E+08	9.94E+07	4.46E+07	6.76E+07	3.19E+07	9.30E+06	4.33E+07	1.21E+07
1100	4.02E+08	2.94E+08	1.31E+08	1.92E+08	1.02E+08	2.91E+07	1.32E+08	3.69E+07
1200	9.34E+08	7.30E+08	3.23E+08	4.61E+08	2.68E+08	7.56E+07	3.38E+08	9.41E+07
1300	1.91E+09	1.58E+09	6.95E+08	9.69E+08	6.12E+08	1.70E+08	7.49E+08	2.09E+08
1400	3.54E+09	3.08E+09	1.34E+09	1.84E+09	1.25E+09	3.43E+08	1.49E+09	4.14E+08
1500	6.06E+09	5.49E+09	2.39E+09	3.21E+09	2.31E+09	6.29E+08	2.70E+09	7.52E+08

Table S20. Rate constants for R1 with boat-ax transition states.

	boat-ax					
T (K)	25	26	27	28	29	30
300	4.11E-06	1.62E-07	3.08E-07	1.90E-05	1.57E-07	5.11E-09
400	1.44E-01	1.98E-02	1.56E-02	3.70E-01	1.03E-02	9.28E-04
500	7.92E+01	2.31E+01	1.06E+01	1.44E+02	8.33E+00	1.38E+00
600	5.45E+03	2.65E+03	8.47E+02	7.89E+03	7.40E+02	1.85E+02
700	1.14E+05	8.00E+04	1.97E+04	1.41E+05	1.86E+04	6.26E+03
800	1.14E+06	1.05E+06	2.12E+05	1.24E+06	2.12E+05	8.94E+04
900	6.86E+06	7.86E+06	1.36E+06	6.81E+06	1.42E+06	7.16E+05
1000	2.91E+07	3.97E+07	6.05E+06	2.69E+07	6.59E+06	3.82E+06
1100	9.58E+07	1.51E+08	2.07E+07	8.31E+07	2.32E+07	1.51E+07
1200	2.59E+08	4.60E+08	5.78E+07	2.14E+08	6.67E+07	4.79E+07
1300	6.05E+08	1.19E+09	1.39E+08	4.79E+08	1.63E+08	1.28E+08
1400	1.26E+09	2.69E+09	2.95E+08	9.57E+08	3.54E+08	2.96E+08
1500	2.37E+09	5.47E+09	5.67E+08	1.75E+09	6.92E+08	6.17E+08

Table S21. Rate constants of every pathway of R2.

	BC-eq	TBC-eq	BC-ax	TBC-ax
T (K)	1	2	3	4
300	3.75E-03	3.34E-03	1.62E-04	1.71E-04
400	1.28E+01	1.51E+01	1.08E+00	1.72E+00
500	1.74E+03	2.44E+03	2.21E+02	4.50E+02
600	4.71E+04	7.46E+04	7.88E+03	1.90E+04
700	5.08E+05	8.76E+05	1.03E+05	2.81E+05
800	3.06E+06	5.65E+06	7.23E+05	2.16E+06
900	1.25E+07	2.43E+07	3.33E+06	1.07E+07
1000	3.91E+07	7.91E+07	1.14E+07	3.87E+07

1100	9.97E+07	2.09E+08	3.13E+07	1.12E+08
1200	2.19E+08	4.71E+08	7.33E+07	2.72E+08
1300	4.27E+08	9.42E+08	1.51E+08	5.80E+08
1400	7.60E+08	1.71E+09	2.81E+08	1.11E+09
1500	1.26E+09	2.88E+09	4.84E+08	1.97E+09

Table S22. Rate constants of every pathway of R3 with chair-eq1-ax2 transition states.

T (K)	1	2	3	4	5	6
300	2.94E-07	6.27E-06	3.03E-07	1.46E-05	1.78E-04	9.69E-06
400	1.12E-02	1.19E-01	1.03E-02	1.82E-01	1.26E+00	1.22E-01
500	6.50E+00	4.53E+01	5.56E+00	5.39E+01	2.63E+02	3.60E+01
600	4.63E+02	2.44E+03	3.78E+02	2.45E+03	9.51E+03	1.64E+03
700	9.96E+03	4.30E+04	7.87E+03	3.83E+04	1.26E+05	2.55E+04
800	1.01E+05	3.75E+05	7.78E+04	3.06E+05	8.85E+05	2.03E+05
900	6.19E+05	2.04E+06	4.68E+05	1.55E+06	4.08E+06	1.03E+06
1000	2.66E+06	8.01E+06	1.99E+06	5.76E+06	1.40E+07	3.83E+06
1100	8.86E+06	2.47E+07	6.52E+06	1.69E+07	3.86E+07	1.12E+07
1200	2.42E+07	6.33E+07	1.76E+07	4.18E+07	9.04E+07	2.77E+07
1300	5.70E+07	1.41E+08	4.11E+07	9.02E+07	1.86E+08	5.98E+07
1400	1.19E+08	2.82E+08	8.53E+07	1.75E+08	3.48E+08	1.16E+08
1500	2.26E+08	5.13E+08	1.61E+08	3.11E+08	5.99E+08	2.06E+08

Table S23. Rate constants of every pathway of R3 with chair-ax1-eq2 transition states.

T (K)	7	8	9	10	11	12	13	14	15
300	7.78E-06	6.95E-07	1.96E-07	8.06E-07	1.19E-07	6.00E-09	9.29E-07	7.71E-08	1.71E-08
400	1.60E-01	2.41E-02	9.31E-03	2.17E-02	6.09E-03	5.50E-04	2.46E-02	4.38E-03	1.31E-03
500	6.42E+01	1.31E+01	6.16E+00	1.02E+01	4.20E+00	5.38E-01	1.15E+01	3.22E+00	1.16E+00
600	3.59E+03	9.01E+02	4.81E+02	6.36E+02	3.37E+02	5.45E+01	7.09E+02	2.70E+02	1.09E+02
700	6.49E+04	1.88E+04	1.10E+04	1.24E+04	7.89E+03	1.50E+03	1.38E+04	6.51E+03	2.87E+03
800	5.79E+05	1.87E+05	1.17E+05	1.17E+05	8.53E+04	1.84E+04	1.30E+05	7.20E+04	3.38E+04
900	3.21E+06	1.12E+06	7.45E+05	6.82E+05	5.49E+05	1.31E+05	7.52E+05	4.72E+05	2.33E+05
1000	1.27E+07	4.77E+06	3.31E+06	2.81E+06	2.46E+06	6.31E+05	3.09E+06	2.14E+06	1.10E+06
1100	3.97E+07	1.57E+07	1.13E+07	9.02E+06	8.44E+06	2.31E+06	9.90E+06	7.44E+06	3.96E+06
1200	1.03E+08	4.25E+07	3.14E+07	2.40E+07	2.37E+07	6.84E+06	2.63E+07	2.11E+07	1.16E+07
1300	2.31E+08	9.91E+07	7.52E+07	5.50E+07	5.70E+07	1.72E+07	6.02E+07	5.12E+07	2.87E+07
1400	4.63E+08	2.05E+08	1.59E+08	1.12E+08	1.21E+08	3.80E+07	1.23E+08	1.10E+08	6.29E+07
1500	8.48E+08	3.88E+08	3.06E+08	2.09E+08	2.34E+08	7.59E+07	2.29E+08	2.13E+08	1.24E+08

Table S24. Rate constants of every pathway of R3 with chair-ax1-ax2 transition states.

T (K)	16	17	18	19	20
300	6.19E-08	2.95E-07	1.12E-06	1.45E-05	5.26E-07
400	4.01E-03	9.77E-03	2.61E-02	2.00E-01	1.37E-02
500	3.18E+00	5.19E+00	1.13E+01	6.26E+01	6.27E+00
600	2.81E+02	3.49E+02	6.61E+02	2.96E+03	3.83E+02
700	7.04E+03	7.22E+03	1.24E+04	4.76E+04	7.37E+03
800	8.01E+04	7.10E+04	1.13E+05	3.88E+05	6.88E+04

900	5.38E+05	4.25E+05	6.39E+05	2.01E+06	3.95E+05
1000	2.49E+06	1.80E+06	2.58E+06	7.54E+06	1.62E+06
1100	8.78E+06	5.89E+06	8.14E+06	2.24E+07	5.15E+06
1200	2.53E+07	1.59E+07	2.13E+07	5.59E+07	1.36E+07
1300	6.20E+07	3.70E+07	4.83E+07	1.22E+08	3.11E+07
1400	1.34E+08	7.67E+07	9.78E+07	2.38E+08	6.33E+07
1500	2.63E+08	1.45E+08	1.81E+08	4.26E+08	1.18E+08

Table S25. Rate constants of every pathway of R3 with chair-eq1-eq2 transition states.

T (K)	21	22	23	24	25	26	27	28
300	8.74E-05	1.05E-05	1.03E-05	9.52E-06	1.54E-06	3.53E-07	2.80E-06	1.24E-07
400	1.01E+00	1.61E-01	1.52E-01	1.72E-01	4.11E-02	1.34E-02	6.95E-02	5.99E-03
500	2.85E+02	5.42E+01	5.02E+01	6.37E+01	1.92E+01	7.70E+00	3.11E+01	4.00E+00
600	1.26E+04	2.69E+03	2.46E+03	3.36E+03	1.18E+03	5.45E+02	1.86E+03	3.13E+02
700	1.92E+05	4.47E+04	4.04E+04	5.82E+04	2.29E+04	1.17E+04	3.53E+04	7.20E+03
800	1.51E+06	3.74E+05	3.35E+05	5.01E+05	2.14E+05	1.17E+05	3.25E+05	7.66E+04
900	7.58E+06	1.97E+06	1.76E+06	2.70E+06	1.23E+06	7.16E+05	1.85E+06	4.88E+05
1000	2.78E+07	7.52E+06	6.68E+06	1.05E+07	5.05E+06	3.07E+06	7.50E+06	2.16E+06
1100	8.10E+07	2.26E+07	2.00E+07	3.21E+07	1.61E+07	1.02E+07	2.37E+07	7.36E+06
1200	1.99E+08	5.70E+07	5.03E+07	8.17E+07	4.26E+07	2.77E+07	6.23E+07	2.05E+07
1300	4.26E+08	1.25E+08	1.10E+08	1.81E+08	9.73E+07	6.49E+07	1.41E+08	4.91E+07
1400	8.22E+08	2.46E+08	2.16E+08	3.59E+08	1.98E+08	1.35E+08	2.87E+08	1.04E+08
1500	1.46E+09	4.44E+08	3.89E+08	6.52E+08	3.68E+08	2.56E+08	5.31E+08	2.00E+08

Table S26. Rate constants of every pathway of R3 with boat-eq1 transition states.

T (K)	29	30	31	32	33	34	35	36
300	8.69E-09	7.83E-08	1.13E-08	4.79E-08	2.08E-07	8.89E-09	7.27E-08	3.87E-07
400	9.41E-04	4.97E-03	1.03E-03	3.52E-03	1.09E-02	1.07E-03	4.19E-03	1.51E-02
500	1.02E+00	3.89E+00	1.01E+00	3.02E+00	7.58E+00	1.23E+00	3.11E+00	8.83E+00
600	1.10E+02	3.39E+02	1.02E+02	2.79E+02	6.11E+02	1.39E+02	2.63E+02	6.35E+02
700	3.18E+03	8.39E+03	2.80E+03	7.21E+03	1.43E+04	4.12E+03	6.38E+03	1.37E+04
800	4.03E+04	9.45E+04	3.41E+04	8.39E+04	1.55E+05	5.33E+04	7.09E+04	1.40E+05
900	2.93E+05	6.28E+05	2.41E+05	5.73E+05	9.97E+05	3.94E+05	4.67E+05	8.58E+05
1000	1.45E+06	2.88E+06	1.16E+06	2.68E+06	4.46E+06	1.97E+06	2.13E+06	3.70E+06
1100	5.38E+06	1.01E+07	4.25E+06	9.56E+06	1.53E+07	7.40E+06	7.42E+06	1.23E+07
1200	1.61E+07	2.88E+07	1.26E+07	2.77E+07	4.29E+07	2.24E+07	2.11E+07	3.37E+07
1300	4.11E+07	7.03E+07	3.16E+07	6.84E+07	1.03E+08	5.74E+07	5.14E+07	7.94E+07
1400	9.18E+07	1.51E+08	6.98E+07	1.49E+08	2.20E+08	1.29E+08	1.10E+08	1.66E+08
1500	1.85E+08	2.95E+08	1.39E+08	2.93E+08	4.24E+08	2.61E+08	2.15E+08	3.15E+08

Table S27. Rate constants of every pathway of R3 with boat-ax1 transition states.

T (K)	37	38	39	40	41	42	43
300	3.52E-09	2.87E-08	5.03E-09	1.82E-08	9.87E-08	1.08E-06	3.52E-09
400	4.47E-04	2.11E-03	5.36E-04	1.57E-03	5.94E-03	3.23E-02	4.47E-04

500	5.33E-01	1.81E+00	5.74E-01	1.49E+00	4.52E+00	1.62E+01	5.33E-01
600	6.15E+01	1.68E+02	6.17E+01	1.47E+02	3.86E+02	1.05E+03	6.15E+01
700	1.87E+03	4.35E+03	1.78E+03	3.99E+03	9.44E+03	2.10E+04	1.87E+03
800	2.45E+04	5.06E+04	2.25E+04	4.82E+04	1.05E+05	2.02E+05	2.45E+04
900	1.84E+05	3.46E+05	1.64E+05	3.39E+05	6.97E+05	1.18E+06	1.84E+05
1000	9.29E+05	1.62E+06	8.07E+05	1.63E+06	3.18E+06	4.93E+06	9.29E+05
1100	3.52E+06	5.79E+06	3.00E+06	5.91E+06	1.11E+07	1.59E+07	3.52E+06
1200	1.08E+07	1.68E+07	9.02E+06	1.74E+07	3.16E+07	4.25E+07	1.08E+07
1300	2.78E+07	4.15E+07	2.30E+07	4.37E+07	7.70E+07	9.80E+07	2.78E+07
1400	6.28E+07	9.04E+07	5.13E+07	9.62E+07	1.66E+08	2.01E+08	6.28E+07
1500	1.28E+08	1.78E+08	1.03E+08	1.91E+08	3.23E+08	3.76E+08	1.28E+08

Table S28. Rate constants of every pathway of R4 with chair-eq1 transition states.

T (K)	1	2	3	4	5	6	7	8	9
300	3.14E-10	2.43E-09	9.30E-11	1.68E-11	2.30E-10	1.01E-11	1.08E-10	7.77E-10	3.37E-11
400	5.20E-05	2.92E-04	1.83E-05	5.48E-06	4.40E-05	4.23E-06	2.28E-05	1.10E-04	9.42E-06
500	7.28E-02	3.36E-01	2.83E-02	1.14E-02	6.68E-02	1.03E-02	3.69E-02	1.39E-01	1.79E-02
600	9.40E+00	3.80E+01	3.91E+00	1.92E+00	9.07E+00	1.92E+00	5.22E+00	1.67E+01	2.83E+00
700	3.10E+02	1.14E+03	1.35E+02	7.64E+01	3.09E+02	8.22E+01	1.84E+02	5.24E+02	1.08E+02
800	4.34E+03	1.49E+04	1.96E+03	1.23E+03	4.44E+03	1.40E+03	2.70E+03	7.05E+03	1.68E+03
900	3.43E+04	1.11E+05	1.59E+04	1.08E+04	3.57E+04	1.29E+04	2.21E+04	5.40E+04	1.44E+04
1000	1.81E+05	5.60E+05	8.56E+04	6.23E+04	1.91E+05	7.67E+04	1.20E+05	2.78E+05	8.08E+04
1100	7.12E+05	2.12E+06	3.43E+05	2.63E+05	7.62E+05	3.33E+05	4.85E+05	1.07E+06	3.35E+05
1200	2.24E+06	6.47E+06	1.09E+06	8.77E+05	2.42E+06	1.14E+06	1.56E+06	3.30E+06	1.10E+06
1300	5.95E+06	1.67E+07	2.94E+06	2.44E+06	6.47E+06	3.24E+06	4.19E+06	8.62E+06	3.03E+06
1400	1.38E+07	3.78E+07	6.87E+06	5.90E+06	1.51E+07	7.96E+06	9.85E+06	1.97E+07	7.23E+06
1500	2.86E+07	7.70E+07	1.44E+07	1.27E+07	3.15E+07	1.74E+07	2.07E+07	4.04E+07	1.54E+07

Table S29. Rate constants of every pathway of R4 with twist-chair transition states.

T (K)	10	11	12	13	14	15	16
300	2.88E-10	2.87E-09	3.56E-10	5.36E-12	1.06E-10	8.15E-09	1.31E-09
400	4.91E-05	2.92E-04	5.99E-05	1.77E-06	1.98E-05	6.23E-04	1.44E-04
500	6.96E-02	3.04E-01	8.44E-02	3.73E-03	2.96E-02	5.47E-01	1.58E-01
600	9.04E+00	3.21E+01	1.09E+01	6.32E-01	3.98E+00	5.16E+01	1.72E+01
700	2.99E+02	9.16E+02	3.61E+02	2.53E+01	1.35E+02	1.36E+03	5.03E+02
800	4.20E+03	1.15E+04	5.06E+03	4.11E+02	1.94E+03	1.61E+04	6.44E+03
900	3.33E+04	8.34E+04	4.00E+04	3.64E+03	1.56E+04	1.11E+05	4.74E+04
1000	1.76E+05	4.11E+05	2.11E+05	2.10E+04	8.34E+04	5.29E+05	2.37E+05
1100	6.92E+05	1.53E+06	8.30E+05	8.91E+04	3.32E+05	1.91E+06	8.88E+05
1200	2.18E+06	4.59E+06	2.61E+06	2.98E+05	1.05E+06	5.59E+06	2.69E+06
1300	5.78E+06	1.17E+07	6.93E+06	8.34E+05	2.82E+06	1.39E+07	6.90E+06
1400	1.34E+07	2.62E+07	1.60E+07	2.02E+06	6.56E+06	3.06E+07	1.55E+07
1500	2.78E+07	5.28E+07	3.33E+07	4.36E+06	1.37E+07	6.08E+07	3.15E+07

Table S30. Rate constants of every pathway of R4 with chair-ax transition states.

T (K)	17	18	19	20	21	22	23
300	4.90E-09	2.71E-10	2.07E-10	1.97E-10	8.51E-12	7.73E-12	7.15E-15
400	3.82E-04	4.27E-05	2.99E-05	3.77E-05	3.22E-06	2.83E-06	1.43E-08
500	3.38E-01	5.78E-02	3.82E-02	5.72E-02	7.33E-03	6.32E-03	8.90E-05
600	3.20E+01	7.26E+00	4.63E+00	7.77E+00	1.31E+00	1.11E+00	3.09E-02
700	8.45E+02	2.35E+02	1.45E+02	2.65E+02	5.41E+01	4.56E+01	2.06E+00
800	1.00E+04	3.24E+03	1.97E+03	3.80E+03	8.98E+02	7.54E+02	4.89E+01
900	6.94E+04	2.53E+04	1.51E+04	3.06E+04	8.10E+03	6.76E+03	5.82E+02
1000	3.30E+05	1.32E+05	7.78E+04	1.64E+05	4.75E+04	3.95E+04	4.26E+03
1100	1.19E+06	5.16E+05	3.00E+05	6.53E+05	2.03E+05	1.69E+05	2.19E+04
1200	3.49E+06	1.61E+06	9.28E+05	2.07E+06	6.88E+05	5.69E+05	8.61E+04
1300	8.70E+06	4.25E+06	2.43E+06	5.55E+06	1.94E+06	1.60E+06	2.76E+05
1400	1.91E+07	9.79E+06	5.55E+06	1.29E+07	4.72E+06	3.90E+06	7.49E+05
1500	3.79E+07	2.02E+07	1.14E+07	2.70E+07	1.03E+07	8.45E+06	1.79E+06

(7) High-pressure limit rate constants of R1-R4 using MS-TST/ZCT

Table S31. Rate constants of R1 using MS-TST/ZCT.

T (K)	chair-eq	boat-eq	chair-ax	boat-ax	total
300	8.60E-04	1.43E-07	1.21E-03	1.55E-07	1.03E-03
400	1.52E+00	2.09E-03	2.00E+00	1.77E-03	2.06E+00
500	1.53E+02	7.91E-01	2.00E+02	5.86E-01	2.33E+02
600	3.57E+03	4.54E+01	4.66E+03	3.09E+01	6.00E+03
700	3.56E+04	8.67E+02	4.61E+04	5.53E+02	6.46E+04
800	2.07E+05	8.22E+03	2.65E+05	5.00E+03	4.01E+05
900	8.39E+05	4.85E+04	1.05E+06	2.84E+04	1.71E+06
1000	2.62E+06	2.04E+05	3.21E+06	1.16E+05	5.55E+06
1100	6.74E+06	6.70E+05	8.11E+06	3.74E+05	1.48E+07
1200	1.50E+07	1.82E+06	1.77E+07	1.00E+06	3.41E+07
1300	2.98E+07	4.29E+06	3.44E+07	2.32E+06	6.96E+07
1400	5.41E+07	8.98E+06	6.13E+07	4.81E+06	1.29E+08
1500	9.12E+07	1.71E+07	1.02E+08	9.10E+06	2.23E+08

Table S32. Rate constants of R2 using MS-TST/ZCT.

T (K)	BC-eq	TBC-eq	BC-ax	TBC-ax	total
300	4.31E-03	5.52E-04	2.77E-05	2.90E-05	6.03E-03
400	2.34E+00	6.37E-01	4.56E-02	7.35E-02	3.99E+00
500	1.10E+02	4.72E+01	4.23E+00	8.76E+00	2.19E+02
600	1.49E+03	8.69E+02	9.07E+01	2.22E+02	3.36E+03
700	9.79E+03	7.15E+03	8.35E+02	2.30E+03	2.45E+04
800	4.10E+04	3.55E+04	4.50E+03	1.36E+04	1.12E+05
900	1.27E+05	1.25E+05	1.70E+04	5.49E+04	3.72E+05
1000	3.15E+05	3.47E+05	4.96E+04	1.70E+05	9.86E+05
1100	6.72E+05	8.07E+05	1.20E+05	4.33E+05	2.22E+06

1200	1.27E+06	1.64E+06	2.54E+05	9.50E+05	4.40E+06
1300	2.20E+06	3.02E+06	4.82E+05	1.86E+06	7.93E+06
1400	3.52E+06	5.12E+06	8.37E+05	3.33E+06	1.32E+07
1500	5.33E+06	8.11E+06	1.36E+06	5.53E+06	2.07E+07

Table S33. Rate constants of R3 using MS-TST/ZCT.

T (K)	chair-eq1-ax2	chair-ax1-eq2	chair-ax1-ax2	chair-eq1-eq2	boat-eq1	boat-ax1	total
300	9.03E-04	2.48E-05	4.89E-05	3.81E-04	2.48E-06	1.03E-05	1.2869E-03
400	1.73E+00	1.41E-01	2.04E-01	1.18E+00	1.95E-02	6.43E-02	3.2886E+00
500	1.87E+02	2.93E+01	3.44E+01	1.70E+02	5.16E+00	1.53E+01	4.5392E+02
600	4.60E+03	1.09E+03	1.12E+03	5.03E+03	2.32E+02	6.45E+02	1.3595E+04
700	4.73E+04	1.50E+04	1.39E+04	5.86E+04	3.68E+03	9.74E+03	1.6439E+05
800	2.79E+05	1.09E+05	9.40E+04	3.78E+05	2.99E+04	7.62E+04	1.1068E+06
900	1.13E+06	5.17E+05	4.20E+05	1.63E+06	1.55E+05	3.82E+05	4.9890E+06
1000	3.48E+06	1.80E+06	1.40E+06	5.28E+06	5.79E+05	1.39E+06	1.6870E+07
1100	8.82E+06	5.02E+06	3.78E+06	1.39E+07	1.71E+06	4.03E+06	4.6092E+07
1200	1.92E+07	1.18E+07	8.64E+06	3.11E+07	4.23E+06	9.76E+06	1.0702E+08
1300	3.72E+07	2.43E+07	1.74E+07	6.17E+07	9.10E+06	2.06E+07	2.1887E+08
1400	6.56E+07	4.50E+07	3.18E+07	1.11E+08	1.75E+07	3.91E+07	4.0461E+08
1500	1.07E+08	7.69E+07	5.35E+07	1.85E+08	3.09E+07	6.81E+07	6.8922E+08

Table S34. Rate constants of R4 using MS-TST/ZCT.

T (K)	chair-eq	twist-chair	chair-ax	total
300	1.10E-08	5.97E-08	2.74E-08	2.09E+04
400	3.55E-04	1.14E-03	5.22E-04	3.44E+05
500	2.07E-01	4.80E-01	2.26E-01	2.08E+06
600	1.54E+01	2.87E+01	1.40E+01	7.41E+06
700	3.46E+02	5.52E+02	2.81E+02	1.94E+07
800	3.65E+03	5.18E+03	2.74E+03	4.16E+07
900	2.31E+04	3.00E+04	1.64E+04	7.83E+07
1000	1.02E+05	1.23E+05	6.97E+04	1.34E+08
1100	3.47E+05	3.95E+05	2.30E+05	2.14E+08
1200	9.64E+05	1.05E+06	6.26E+05	3.23E+08
1300	2.30E+06	2.40E+06	1.47E+06	4.67E+08
1400	4.84E+06	4.88E+06	3.05E+06	6.52E+08
1500	9.23E+06	9.04E+06	5.77E+06	8.84E+08

(8) The pressure dependent rate constants of R1-R4.

Table S35. Pressure dependent rate constants of R1.

T(K) \ Pa(bar)	0.1	1	10	100
300	9.83E-04	1.02E-03	1.03E-03	1.03E-03
400	1.70E+00	2.02E+00	2.06E+00	2.06E+00
500	1.52E+02	2.21E+02	2.32E+02	2.33E+02

600	2.82E+03	5.33E+03	5.92E+03	5.98E+03
700	2.03E+04	5.19E+04	6.31E+04	6.46E+04
800	7.82E+04	2.73E+05	3.82E+05	3.99E+05
900	2.13E+05	9.55E+05	1.57E+06	1.69E+06
1000	4.51E+05	2.47E+06	4.89E+06	5.48E+06
1100	8.07E+05	5.15E+06	1.23E+07	1.45E+07
1200	1.28E+06	9.16E+06	2.62E+07	3.31E+07
1300	1.87E+06	1.45E+07	4.89E+07	6.66E+07
1400	2.55E+06	2.09E+07	8.22E+07	1.22E+08
1500	3.30E+06	2.84E+07	1.27E+08	2.06E+08

Table S36. Pressure dependent rate constants of R2.

Pa(bar) / T(K)	0.1	1	10	100
300	6.00E-03	6.04E-03	6.04E-03	6.04E-03
400	3.89E+00	3.96E+00	3.97E+00	3.97E+00
500	2.10E+02	2.19E+02	2.20E+02	2.20E+02
600	3.07E+03	3.33E+03	3.36E+03	3.37E+03
700	2.08E+04	2.40E+04	2.44E+04	2.45E+04
800	8.52E+04	1.09E+05	1.12E+05	1.12E+05
900	2.48E+05	3.53E+05	3.69E+05	3.71E+05
1000	5.66E+05	9.15E+05	9.80E+05	9.87E+05
1100	1.08E+06	1.99E+06	2.19E+06	2.21E+06
1200	1.79E+06	3.81E+06	4.34E+06	4.40E+06
1300	2.69E+06	6.56E+06	7.76E+06	7.91E+06
1400	3.74E+06	1.04E+07	1.28E+07	1.32E+07
1500	4.90E+06	1.54E+07	2.00E+07	2.07E+07

Table S37. Pressure dependent rate constants of R3.

Pa(bar) / T(K)	0.1	1	10	100
300	5.08E-04	1.11E-03	1.27E-03	1.29E-03
400	1.17E+00	2.73E+00	3.21E+00	3.27E+00
500	1.23E+02	3.44E+02	4.37E+02	4.50E+02
600	2.39E+03	8.77E+03	1.28E+04	1.35E+04
700	1.72E+04	8.30E+04	1.48E+05	1.62E+05
800	6.59E+04	4.02E+05	9.22E+05	1.08E+06
900	1.80E+05	1.28E+06	3.74E+06	4.80E+06
1000	3.85E+05	3.06E+06	1.12E+07	1.61E+07
1100	6.97E+05	5.94E+06	2.63E+07	4.26E+07
1200	1.12E+06	1.00E+07	5.19E+07	9.61E+07
1300	1.65E+06	1.52E+07	8.94E+07	1.89E+08
1400	2.27E+06	2.14E+07	1.39E+08	3.34E+08
1500	2.98E+06	2.84E+07	1.99E+08	5.44E+08

Table S38. Pressure dependent rate constants of R3.

T(K) \ Pa(bar)	0.1	1	10	100
300	9.37E-09	3.70E-08	5.28E-08	5.52E-08
400	2.35E-04	8.80E-04	1.24E-03	1.29E-03
500	1.11E-01	4.26E-01	6.14E-01	6.44E-01
600	6.11E+00	2.66E+01	4.17E+01	4.44E+01
700	9.68E+01	4.94E+02	8.87E+02	9.69E+02
800	6.87E+02	4.15E+03	8.92E+03	1.02E+04
900	3.09E+03	2.11E+04	5.43E+04	6.55E+04
1000	9.89E+03	7.44E+04	2.29E+05	2.95E+05
1100	2.50E+04	2.02E+05	7.32E+05	1.02E+06
1200	5.31E+04	4.51E+05	1.90E+06	2.90E+06
1300	9.93E+04	8.75E+05	4.19E+06	7.02E+06
1400	1.68E+05	1.52E+06	8.14E+06	1.51E+07
1500	2.63E+05	2.43E+06	1.43E+07	2.92E+07

(9) Cartesian coordinates of the reactant, products and transition states at M06-2X/6-311++g(d,p)

Table S39. Cartesian coordinates of the reactants.

Reactant 1				Reactant 2			
C	-2.72354	1.099441	0.106007	C	2.849802	0.116529	2.664567
H	-3.3931	0.937751	-0.74022	H	2.10429	0.27965	3.443743
H	-1.96712	1.832784	-0.17782	H	2.972901	1.041393	2.099858
H	-3.30351	1.497539	0.940603	H	3.799876	-0.13403	3.139118
C	-2.05345	-0.19528	0.505325	C	2.414966	-1.00685	1.751012
H	-1.35409	-0.0293	1.329176	H	3.150031	-1.17702	0.955086
H	-2.78622	-0.95249	0.812107	H	2.280489	-1.94027	2.303899
O	-1.34122	-0.68507	-0.63232	O	1.17122	-0.62565	1.157002
C	-0.44667	-1.69484	-0.34529	C	0.705298	-1.49247	0.211509
H	-0.11534	-2.09955	-1.30562	H	1.45464	-1.82349	-0.51329
H	-0.88499	-2.47954	0.279223	O	-0.35682	-0.99262	-0.45694
O	0.681969	-1.2433	0.392775	C	-1.40948	-0.4461	0.356301
C	1.373684	-0.20724	-0.19171	H	-1.68356	-1.17448	1.124129
H	1.269488	-0.19459	-1.28178	C	-2.57062	-0.15319	-0.56633
C	2.804234	-0.19628	0.278624	H	-2.91515	-1.06881	-1.04829
H	3.31349	-1.08588	-0.09233	H	-3.39751	0.277674	0.000873
H	3.307681	0.694353	-0.09678	H	-2.27174	0.555866	-1.3396
H	2.82448	-0.20009	1.369104	H	-1.04375	0.458078	0.846173
O	0.718449	1.03008	0.266209	O	0.312542	-2.71192	0.957304
O	1.111262	2.053805	-0.42085	O	0.23429	-3.73497	0.163164
E_{0K}= -496.6697664				E_{0K}=-496.6708106			

Table S40. Cartesian coordinates of the products.

Product 1 (P1)				Product 2 (P2)			
C	2.743558	1.130921	-0.0471	C	-2.17665	-0.59187	1.087072
H	2.19508	1.477351	0.830534	H	-2.80209	0.106987	1.651256
H	2.331537	1.628291	-0.9269	H	-1.24988	-0.76607	1.636705
H	3.790125	1.423727	0.061442	H	-2.69737	-1.54706	1.010261
C	2.64438	-0.37616	-0.20161	C	-1.92403	-0.05518	-0.30212
H	3.204709	-0.72236	-1.06963	H	-1.05272	-0.87819	-0.79025
H	3.036467	-0.88965	0.684438	H	-2.77442	-0.12452	-0.97989
O	1.300303	-0.81109	-0.43358	O	-1.41715	1.227518	-0.39558
C	0.458651	-0.68346	0.635685	C	-0.14291	1.462407	0.150252
H	0.922564	-0.85889	1.609467	H	-0.05805	1.023519	1.14922
H	-0.49904	-1.57474	0.374251	H	-0.04868	2.54544	0.19386
O	-0.28028	0.479127	0.671638	O	0.853933	0.975715	-0.70541
C	-1.33569	0.492847	-0.28987	C	1.58356	-0.16115	-0.30453
H	-0.91819	0.308042	-1.28372	H	2.088766	-0.48866	-1.21441
C	-2.08882	1.786515	-0.15915	C	2.550776	0.110176	0.829028
H	-1.41593	2.619499	-0.36065	H	3.14335	-0.78117	1.034615
H	-2.9125	1.806249	-0.87199	H	3.212834	0.926893	0.542291
H	-2.48057	1.877534	0.854056	H	2.01715	0.387243	1.740181
O	-2.19916	-0.56239	0.046581	O	0.736209	-1.19608	0.149681
O	-1.54421	-1.75553	-0.22577	O	-0.06341	-1.63099	-0.8902
E_{0K}= -496.6511837				E_{0K}= -496.6539987			

Product 3 (P3)				Product 4 (P4)			
C	2.788949	0.383976	2.564944	C	-2.23637	-1.77815	-0.34242
H	2.042045	0.603801	3.328823	H	-1.81813	-2.56107	-0.97701
H	2.896801	1.258145	1.921727	H	-2.59629	-0.96732	-0.97834
H	3.743303	0.189767	3.057315	H	-3.08014	-2.19254	0.211978
C	2.369123	-0.82129	1.753992	C	-1.18811	-1.25248	0.612268
H	3.105988	-1.04829	0.973608	H	-1.59636	-0.4438	1.22704
H	2.250726	-1.70605	2.38395	H	-0.81721	-2.042	1.276579
O	1.119777	-0.50893	1.132844	O	-0.10259	-0.75096	-0.16524
C	0.682588	-1.45508	0.24212	C	0.797229	0.022085	0.564016
H	1.440214	-1.7515	-0.49009	H	1.037793	-0.44359	1.525612
O	-0.39274	-0.96298	-0.47992	O	0.351867	1.294844	0.814056
C	-1.54725	-0.73307	0.231451	C	-0.16496	1.997656	-0.32957
C	-2.58465	-0.01132	-0.54403	H	0.174683	3.031007	-0.19535
H	-2.75333	-0.49739	-1.50802	C	-1.64775	1.92212	-0.38887
H	-3.52431	0.008141	0.00863	H	-2.21994	2.050488	0.520673
H	-2.28635	1.025985	-0.74726	H	-2.15762	1.99554	-1.33958
H	-1.42755	-0.60439	1.300718	H	1.878562	-1.56398	-1.02202
O	0.311865	-2.57591	1.022814	H	0.290016	1.615687	-1.2451
O	-0.0731	-3.60724	0.135825	O	1.954668	0.131739	-0.22824
H	-1.01269	-3.41174	-0.00125	O	2.489106	-1.16885	-0.38271

E_{0K}= -496.6516066	E_{0K}= -496.6405745

Table S41. Cartesian coordinates of the transition state 1 (TS1) within chair-eq structures.

Structure 1				Structure 2			
C	3.813945	-0.32235	-0.49431	C	3.415895	-0.34562	-0.63248
H	3.641879	-0.19283	-1.56317	H	3.832387	-1.09476	0.042306
H	3.92804	-1.38678	-0.28639	H	3.856804	0.622647	-0.3927
H	4.738699	0.189539	-0.2233	H	3.687732	-0.60979	-1.65584
C	2.656147	0.246009	0.294714	C	1.911455	-0.29343	-0.49703
H	2.811867	0.119066	1.373092	H	1.469702	0.470021	-1.14709
H	2.52435	1.314586	0.089375	H	1.450318	-1.25425	-0.73405
O	1.477353	-0.45274	-0.09537	O	1.612575	0.044228	0.865855
C	0.362541	-0.04644	0.561126	C	0.317446	0.337093	1.110715
H	-0.05541	1.137853	0.213798	H	-0.10073	1.362868	0.417619
H	0.496931	0.054353	1.65275	H	0.184511	0.620046	2.15896
O	-0.68885	-0.8522	0.211903	O	-0.55082	-0.65923	0.689566
C	-1.95239	-0.20295	0.266881	C	-1.79278	-0.19066	0.183363
H	-2.1376	0.150925	1.288129	H	-2.33092	0.350898	0.969489
C	-2.99425	-1.1577	-0.24655	C	-2.55	-1.36445	-0.37363
H	-3.00214	-2.05398	0.372685	H	-2.71422	-2.0981	0.414829
H	-3.97474	-0.68412	-0.21365	H	-3.51012	-1.0305	-0.76531
H	-2.75436	-1.43322	-1.27347	H	-1.96864	-1.82243	-1.17424
O	-1.90223	0.908596	-0.58619	O	-1.51911	0.702838	-0.86367
O	-1.07796	1.856988	0.004526	O	-1.00126	1.865376	-0.30171
E_{0K}= -496.6277879				E_{0K}= -496.6324252			

Structure 3				Structure 4			
C	-3.76999	0.232338	-0.44848	C	3.536973	-0.54322	0.487573
H	-4.1708	-0.75513	-0.2166	H	3.684553	-1.49953	-0.01554
H	-3.60255	0.295823	-1.52416	H	3.051048	-0.72922	1.447291
H	-4.5061	0.986036	-0.16332	H	4.513986	-0.09774	0.68503
C	-2.47482	0.464087	0.294667	C	2.711485	0.384076	-0.38775
H	-2.04887	1.444452	0.064033	H	2.551843	1.355685	0.092864
H	-2.61706	0.390835	1.38005	H	3.208038	0.560814	-1.34108
O	-1.54732	-0.55079	-0.11742	O	1.450734	-0.19559	-0.72412
C	-0.3554	-0.5061	0.51727	C	0.480197	0.007237	0.202206
H	0.447464	-1.49668	0.137439	H	-0.0586	1.186828	0.148006
H	-0.40795	-0.64523	1.609703	H	0.827994	-0.05111	1.247602
O	0.391549	0.602279	0.164172	O	-0.57896	-0.82148	-0.06331
C	1.79074	0.399165	0.283093	C	-1.8346	-0.30048	0.351737
H	2.034545	0.108548	1.312144	H	-1.81969	-0.12963	1.434967
C	2.500471	1.638528	-0.18649	C	-2.90964	-1.2493	-0.10097
H	2.203967	2.484415	0.432882	H	-2.73998	-2.22951	0.343183

H	3.5779	1.495537	-0.11255	H	-3.88463	-0.87395	0.207671
H	2.228624	1.838296	-1.22295	H	-2.87757	-1.33716	-1.18691
O	2.130382	-0.66122	-0.57313	O	-2.02372	0.931726	-0.28959
O	1.614731	-1.82965	-0.03075	O	-1.14349	1.842169	0.279532
E_{0K}= -496.6256907				E_{0K}= -496.6256508			

Structure 5				Structure 6			
C	-2.05347	0.797328	1.113073	C	3.094762	0.785307	-0.13813
H	-2.58514	1.512531	0.482383	H	2.53322	1.417046	0.553264
H	-1.01075	1.107915	1.196487	H	2.878462	1.113188	-1.15617
H	-2.49609	0.821902	2.110949	H	4.158042	0.934255	0.058747
C	-2.17824	-0.60662	0.548851	C	2.742868	-0.68424	0.024295
H	-1.5825	-1.31851	1.123298	H	3.366904	-1.3067	-0.61524
H	-3.21518	-0.93933	0.543771	H	2.880515	-1.01242	1.061975
O	-1.78909	-0.68161	-0.83172	O	1.40797	-0.97248	-0.38422
C	-0.51477	-0.3453	-1.12465	C	0.452279	-0.42802	0.409525
H	-0.22851	0.914615	-0.98232	H	0.271522	0.839982	0.230249
H	-0.31932	-0.52626	-2.18684	H	0.679945	-0.49547	1.488957
O	0.410615	-0.94045	-0.28076	O	-0.76837	-0.9532	0.072729
C	1.627081	-0.22004	-0.15862	C	-1.85778	-0.07079	0.308547
H	2.090854	-0.11245	-1.14609	H	-1.89707	0.185238	1.374137
C	2.496169	-0.92017	0.849261	C	-3.11032	-0.72226	-0.20868
H	2.697455	-1.93651	0.512537	H	-3.26804	-1.66794	0.308656
H	3.43644	-0.38142	0.960639	H	-3.96332	-0.06679	-0.03693
H	1.980568	-0.95528	1.809299	H	-3.00228	-0.91131	-1.27667
O	1.320383	1.06118	0.328405	O	-1.62826	1.103809	-0.42227
O	0.679535	1.758578	-0.68989	O	-0.58243	1.78324	0.188221
E_{0K}= -496.6318822				E_{0K}= -496.626901			

Structure 7				Structure 8			
C	-2.51065	1.263925	-0.45678	C	-3.02974	0.740368	0.507932
H	-1.69381	1.877532	-0.07736	H	-2.27055	1.230786	1.120847
H	-3.34981	1.325921	0.237893	H	-3.55556	0.002313	1.116393
H	-2.8319	1.657417	-1.42377	H	-3.74586	1.500705	0.190202
C	-2.0638	-0.17651	-0.61164	C	-2.4069	0.083142	-0.7107
H	-2.87091	-0.79923	-0.99924	H	-3.16493	-0.38036	-1.34019
H	-1.20399	-0.2599	-1.28223	H	-1.84758	0.805677	-1.30754
O	-1.72267	-0.74794	0.664034	O	-1.53926	-1.00382	-0.35146
C	-0.40306	-0.82553	0.935074	C	-0.45971	-0.70203	0.410155
H	0.241808	-1.57977	0.093158	H	0.505786	-1.56936	0.219764
H	-0.24467	-1.28824	1.913672	H	-0.62784	-0.77889	1.496482
O	0.252327	0.389242	0.781232	O	0.145444	0.486038	0.051286
C	1.587144	0.287935	0.3056	C	1.541405	0.512433	0.321602
H	2.19086	-0.28585	1.017669	H	1.70806	0.33453	1.390739

C	2.103542	1.677077	0.049797	C	2.101527	1.816039	-0.17598
H	2.077169	2.251224	0.975306	H	1.610577	2.642988	0.336057
H	3.127798	1.627239	-0.3179	H	3.172513	1.853885	0.019634
H	1.472786	2.165435	-0.6937	H	1.923987	1.899409	-1.24826
O	1.555064	-0.4084	-0.91259	O	2.126976	-0.53406	-0.40363
O	1.265976	-1.73956	-0.62966	O	1.743328	-1.72834	0.189779
E_{0K}= -496.6312062				E_{0K}=-496.6237745			

Table S42. Cartesian coordinates of the transition state 1 (TS1) within boat-eq structures.

Structure 9				Structure 10			
C	-3.84588	-0.31422	0.365927	C	3.361123	0.478068	0.325631
H	-3.71337	-0.62153	1.403697	H	3.820992	0.370359	-0.65751
H	-4.01731	-1.20367	-0.24129	H	3.72937	-0.31994	0.971301
H	-4.72415	0.329993	0.300582	H	3.662728	1.437796	0.748518
C	-2.62191	0.427082	-0.1221	C	1.854984	0.414043	0.209934
H	-2.73801	0.7385	-1.16706	H	1.37368	0.504131	1.191352
H	-2.4316	1.32044	0.483585	H	1.46785	1.202663	-0.44028
O	-1.50705	-0.45497	-0.01699	O	1.517569	-0.85886	-0.34485
C	-0.34356	0.089936	-0.44497	C	0.192988	-1.12099	-0.4686
H	0.136502	0.99877	0.334174	H	-0.39383	-1.15167	0.687744
H	-0.41939	0.631474	-1.40452	H	0.062222	-2.11767	-0.89471
O	0.632339	-0.8693	-0.4137	O	-0.5168	-0.14723	-1.15528
C	1.97652	-0.38631	-0.45411	C	-1.70223	0.395957	-0.55874
H	2.399055	-0.61696	-1.43546	H	-2.43954	0.457767	-1.35997
C	2.744605	-1.02492	0.676837	C	-1.42566	1.747977	0.06027
H	2.657839	-2.10927	0.606941	H	-0.98928	2.40496	-0.69283
H	3.794844	-0.73895	0.61114	H	-2.36305	2.180235	0.413045
H	2.332042	-0.69136	1.628138	H	-0.74165	1.653413	0.901908
O	1.992612	1.02305	-0.42197	O	-2.25461	-0.532	0.335483
O	1.290218	1.452866	0.696472	O	-1.35575	-0.72597	1.379696
E_{0K}=-496.6201575				E_{0K}=-496.6232241			

Structure 11				Structure 12			
C	3.801852	0.22398	0.340397	C	3.518591	-0.16138	0.616667
H	4.149377	-0.80945	0.367248	H	3.745222	-1.22614	0.550777
H	3.690279	0.580217	1.365082	H	3.007949	0.025861	1.563152
H	4.554102	0.834391	-0.16235	H	4.45728	0.396132	0.62322
C	2.483073	0.319283	-0.39114	C	2.670592	0.265696	-0.5687
H	2.110258	1.346448	-0.41831	H	2.43179	1.334175	-0.52866
H	2.568774	-0.04947	-1.42071	H	3.189818	0.072845	-1.50677
O	1.534653	-0.49783	0.311847	O	1.461453	-0.4909	-0.647
C	0.323206	-0.58208	-0.27878	C	0.446893	0.011586	0.09768
H	-0.50511	-1.33319	0.410144	H	-0.14377	1.018469	-0.43672
H	0.314219	-1.07526	-1.2644	H	0.749489	0.420949	1.076668

O	-0.34209	0.6283	-0.26661	O	-0.55479	-0.91999	0.166091
C	-1.75106	0.563074	-0.48028	C	-1.83985	-0.42247	0.545466
H	-1.97538	0.913479	-1.4913	H	-2.06381	-0.77929	1.553995
C	-2.43129	1.382941	0.588366	C	-2.85052	-0.8864	-0.47458
H	-2.03034	2.396667	0.580321	H	-2.80336	-1.97185	-0.56318
H	-3.50404	1.415257	0.39584	H	-3.85086	-0.59036	-0.15702
H	-2.24615	0.930103	1.561782	H	-2.62374	-0.4364	-1.44019
O	-2.17545	-0.78345	-0.50915	O	-1.79758	0.977482	0.702478
O	-1.72721	-1.42106	0.639563	O	-1.33037	1.545077	-0.47588
E_{0K}=-496.6182122				E_{0K}=-496.6182206			

Structure 13				Structure 14			
C	-2.08008	1.083534	-0.88611	C	-3.00497	0.894551	0.391568
H	-2.48558	0.492792	-1.70991	H	-2.36238	1.628181	-0.09953
H	-1.01902	1.260417	-1.07172	H	-2.81953	0.935575	1.466242
H	-2.58861	2.049428	-0.87059	H	-4.04259	1.178654	0.206712
C	-2.30391	0.375163	0.438292	C	-2.75674	-0.51118	-0.12936
H	-1.85202	0.927534	1.264105	H	-3.44803	-1.22159	0.321627
H	-3.36611	0.244927	0.639822	H	-2.87889	-0.55707	-1.21821
O	-1.78724	-0.96334	0.432847	O	-1.46218	-0.99936	0.216284
C	-0.45966	-1.09898	0.228964	C	-0.44268	-0.36135	-0.40841
H	-0.05991	-0.80264	-0.96046	H	-0.16904	0.791599	0.070421
H	-0.16658	-2.14876	0.332205	H	-0.64021	-0.13145	-1.47118
O	0.2836	-0.21469	0.993663	O	0.715655	-1.05848	-0.18686
C	1.642106	-0.0228	0.601542	C	1.931768	-0.32931	-0.37421
H	2.288257	-0.52322	1.327503	H	2.436235	-0.72753	-1.25796
C	1.909601	1.460166	0.511816	C	2.764019	-0.45734	0.878321
H	1.640726	1.937097	1.454722	H	2.912744	-1.51273	1.106848
H	2.967716	1.629091	0.309768	H	3.731613	0.021204	0.723337
H	1.313929	1.889301	-0.29356	H	2.247173	0.021111	1.709075
O	1.908965	-0.71512	-0.59683	O	1.655487	1.003921	-0.73559
O	0.979538	-0.32417	-1.5533	O	0.851612	1.574142	0.243067
E_{0K}=-496.6234147				E_{0K}=-496.6193136			

Structure 15				Structure 16			
C	2.750306	1.054719	0.018858	C	-3.04577	0.500171	0.729847
H	2.008268	1.611341	-0.55265	H	-2.27463	0.850359	1.419238
H	3.548521	0.736976	-0.65372	H	-3.50149	-0.40433	1.136666
H	3.180168	1.710436	0.779473	H	-3.81239	1.274579	0.663193
C	2.115002	-0.15218	0.681741	C	-2.46614	0.234548	-0.64768
H	2.848105	-0.70906	1.266517	H	-3.23794	-0.08595	-1.34582
H	1.292166	0.140562	1.34042	H	-1.97484	1.122652	-1.04881
O	1.624655	-1.08325	-0.29556	O	-1.53073	-0.8562	-0.63572
C	0.299469	-1.03432	-0.54672	C	-0.42781	-0.7101	0.134578

H	-0.42255	-1.35387	0.47132	H	0.547529	-1.45303	-0.29372
H	0.029463	-1.77062	-1.30968	H	-0.5296	-1.06608	1.172352
O	-0.13887	0.255359	-0.81103	O	0.120084	0.552875	0.038975
C	-1.51816	0.542096	-0.57062	C	1.476636	0.669981	0.472585
H	-1.99974	0.733621	-1.53244	H	1.496745	1.182408	1.438019
C	-1.60669	1.722343	0.367594	C	2.252651	1.401963	-0.59475
H	-1.04366	2.558989	-0.04725	H	1.772827	2.358297	-0.80401
H	-2.64995	2.014741	0.491441	H	3.271858	1.576163	-0.24859
H	-1.18974	1.450072	1.33693	H	2.27132	0.800509	-1.50285
O	-2.18392	-0.60391	-0.09813	O	1.999965	-0.60361	0.774285
O	-1.53194	-1.05809	1.042791	O	1.814823	-1.43493	-0.32169
E_{0K}=-496.6225924				E_{0K}=-496.6164734			

Table S43. Cartesian coordinates of the transition state 1 (TS1) within chair-ax structures.

Structure 17				Structure 18			
C	-3.47389	-0.36917	-0.75062	C	3.458083	0.337821	-0.7172
H	-3.69873	-1.39153	-0.44459	H	3.047637	0.651343	-1.67783
H	-3.08819	-0.387	-1.77059	H	3.848999	-0.67494	-0.8214
H	-4.39719	0.212164	-0.73685	H	4.27969	1.005994	-0.453
C	-2.45666	0.249395	0.181649	C	2.388545	0.380832	0.350186
H	-2.21693	1.276639	-0.1163	H	2.784892	0.064631	1.322712
H	-2.82768	0.268033	1.214132	H	1.969947	1.386519	0.459111
O	-1.2696	-0.53621	0.122661	O	1.343229	-0.51936	-0.03806
C	-0.29971	-0.12064	0.998144	C	0.310453	-0.58465	0.854982
H	-0.58931	-0.16051	2.053091	H	-0.46875	-1.54954	0.340338
H	0.003615	1.115408	0.64704	H	0.601717	-0.80433	1.885411
O	0.883527	-0.76074	0.787264	O	-0.55277	0.487474	0.83133
C	1.570069	-0.28174	-0.37433	C	-1.41603	0.476206	-0.3077
H	0.904795	-0.36486	-1.23793	H	-0.8101	0.428053	-1.21696
C	2.862575	-1.03624	-0.50645	C	-2.33332	1.663697	-0.22844
H	2.650175	-2.0982	-0.62434	H	-1.74318	2.579534	-0.23925
H	3.410601	-0.67708	-1.37679	H	-3.01263	1.661215	-1.08016
H	3.463503	-0.88678	0.390686	H	-2.90762	1.617056	0.696906
O	1.862812	1.070496	-0.14666	O	-2.18862	-0.69159	-0.21178
O	0.66964	1.781955	-0.17426	O	-1.35647	-1.77765	-0.44735
E_{0K}=-496.6310722				E_{0K}=-496.6281164			

Structure 19				Structure 20			
C	3.413438	0.104352	0.333931	C	-2.84222	0.815755	-0.3508
H	3.109922	-0.27716	1.310545	H	-2.42594	1.150462	-1.30183
H	3.644864	1.167069	0.427013	H	-2.40773	1.42354	0.444772
H	4.323592	-0.42318	0.042711	H	-3.91993	0.990846	-0.35789
C	2.341003	-0.11304	-0.7216	C	-2.56951	-0.66688	-0.15244
H	2.703138	0.186923	-1.70417	H	-2.91336	-1.00466	0.833179

H	2.041522	-1.16614	-0.77295	H	-3.08251	-1.25888	-0.90954
O	1.176616	0.683872	-0.50816	O	-1.19058	-0.99639	-0.30478
C	0.470949	0.380546	0.628793	C	-0.39927	-0.62243	0.750005
H	0.9618	0.638528	1.570314	H	-0.7499	-0.97882	1.724582
H	0.223717	-0.91934	0.564832	H	-0.3303	0.686009	0.74014
O	-0.78982	0.896437	0.588985	O	0.906621	-0.95661	0.544582
C	-1.65141	0.177751	-0.2986	C	1.572469	-0.07118	-0.36149
H	-1.19273	0.145695	-1.29037	H	1.012632	-0.03817	-1.30021
C	-3.01211	0.813724	-0.26022	C	2.999064	-0.52138	-0.501
H	-2.93664	1.847432	-0.59569	H	3.020527	-1.5334	-0.90361
H	-3.69123	0.268679	-0.91488	H	3.531848	0.148704	-1.17477
H	-3.39402	0.793553	0.760576	H	3.479364	-0.5131	0.47757
O	-1.75419	-1.12813	0.204593	O	1.560365	1.202278	0.225506
O	-0.52825	-1.75743	0.028106	O	0.251356	1.666244	0.212425
E_{0K}=-496.6287097				E_{0K}=-496.6297981			

Structure 21				Structure 22			
C	-3.15032	0.505312	-0.4002	C	-2.22283	-1.38487	-0.49689
H	-3.67384	-0.41337	-0.67177	H	-2.97585	-1.63288	0.252487
H	-2.62694	0.887983	-1.27869	H	-1.28925	-1.87042	-0.21207
H	-3.891	1.250062	-0.10294	H	-2.54934	-1.78314	-1.46018
C	-2.19268	0.251824	0.750146	C	-2.06895	0.123756	-0.59428
H	-1.61594	1.152702	0.980585	H	-1.31598	0.418404	-1.33108
H	-2.72835	-0.05487	1.647573	H	-3.01552	0.580715	-0.88364
O	-1.28917	-0.83252	0.489693	O	-1.7462	0.714642	0.669813
C	-0.4797	-0.68456	-0.60391	C	-0.43249	0.847519	0.992974
H	-0.95241	-0.8724	-1.57019	H	-0.35737	1.329207	1.966665
H	0.488484	-1.57627	-0.37637	H	0.17137	1.607124	0.11298
O	0.241733	0.485518	-0.64927	O	0.34797	-0.29768	0.955881
C	1.342366	0.492911	0.26556	C	1.187687	-0.4806	-0.18627
H	0.971473	0.288398	1.27479	H	0.572146	-0.70411	-1.06349
C	2.076659	1.795926	0.12138	C	2.17962	-1.56369	0.136837
H	1.405027	2.619892	0.361166	H	1.645763	-2.48311	0.376528
H	2.928895	1.815378	0.79974	H	2.83061	-1.73482	-0.72
H	2.42483	1.903806	-0.90591	H	2.776462	-1.26202	0.997519
O	2.194275	-0.54853	-0.12545	O	1.886883	0.708456	-0.41992
O	1.564636	-1.75069	0.165551	O	0.967435	1.659884	-0.84953
E_{0K}=-496.6256185				E_{0K}=-496.6264724			

Structure 23				Structure 24			
C	2.743558	1.130921	-0.0471	C	2.311044	0.710573	1.078133
H	2.19508	1.477351	0.830534	H	1.418689	1.337278	1.041527
H	2.331537	1.628291	-0.9269	H	3.100184	1.197628	0.503149
H	3.790125	1.423727	0.061442	H	2.637807	0.634274	2.117578

C	2.64438	-0.37616	-0.20161	C	2.046576	-0.68052	0.525913
H	3.204709	-0.72236	-1.06963	H	2.947021	-1.29197	0.576903
H	3.036467	-0.88965	0.684438	H	1.257074	-1.19855	1.077369
O	1.300303	-0.81109	-0.43358	O	1.713701	-0.6533	-0.86307
C	0.458651	-0.68346	0.635685	C	0.443095	-0.31136	-1.21333
H	0.922564	-0.85889	1.609467	H	0.33121	-0.45456	-2.2879
H	-0.49904	-1.57474	0.374251	H	0.181492	0.946089	-0.99109
O	-0.28028	0.479127	0.671638	O	-0.57177	-0.94473	-0.51568
C	-1.33569	0.492847	-0.28987	C	-1.30003	-0.14858	0.423925
H	-0.91819	0.308042	-1.28372	H	-0.65246	0.088597	1.27527
C	-2.08882	1.786515	-0.15915	C	-2.54487	-0.90194	0.8029
H	-1.41593	2.619499	-0.36065	H	-2.26994	-1.86612	1.22939
H	-2.9125	1.806249	-0.87199	H	-3.11376	-0.32932	1.534733
H	-2.48057	1.877534	0.854056	H	-3.1521	-1.06491	-0.08751
O	-2.19916	-0.56239	0.046581	O	-1.67389	1.046788	-0.19675
O	-1.54421	-1.75553	-0.22577	O	-0.52056	1.800295	-0.38634
E_{0K}=-496.6270238				E_{0K}=-496.6272368			

Table S44. Cartesian coordinates of the transition state 1 (TS1) within boat-ax structures.

Structure 25				Structure 26			
C	-3.46191	0.103382	-0.67194	C	-3.43121	-0.07512	-0.67374
H	-3.75017	-0.93197	-0.85768	H	-3.09034	0.263776	-1.65273
H	-3.10548	0.539704	-1.6056	H	-3.92527	0.757554	-0.1719
H	-4.34102	0.657941	-0.33978	H	-4.15469	-0.88052	-0.81299
C	-2.3776	0.17045	0.37965	C	-2.25871	-0.5645	0.145139
H	-2.0724	1.204794	0.573032	H	-2.57581	-0.89397	1.142231
H	-2.71381	-0.27393	1.325055	H	-1.74886	-1.39935	-0.34418
O	-1.24883	-0.55183	-0.10561	O	-1.34349	0.529764	0.286839
C	-0.23441	-0.65973	0.802129	C	-0.24922	0.265467	1.053746
H	-0.48671	-1.21664	1.710595	H	-0.44282	0.180178	2.127195
H	0.144891	0.554468	1.13734	H	0.571076	1.291251	0.827114
O	0.907864	-1.14278	0.246322	O	0.53534	-0.78789	0.651489
C	1.599196	-0.24313	-0.63792	C	1.369263	-0.57822	-0.50115
H	1.409471	-0.54715	-1.66927	H	0.964275	-1.15057	-1.33929
C	3.061183	-0.27485	-0.26699	C	2.775102	-0.98821	-0.13528
H	3.421542	-1.30345	-0.29265	H	2.770881	-2.01492	0.231152
H	3.63092	0.326118	-0.97627	H	3.416065	-0.91971	-1.0148
H	3.187723	0.126936	0.737947	H	3.153253	-0.3289	0.645322
O	1.03072	1.042565	-0.57007	O	1.265729	0.752448	-0.93881
O	0.954782	1.437837	0.757822	O	1.521276	1.598013	0.129299
E_{0K}=-496.6245594				E_{0K}=-496.6193651			

Structure 27				Structure 28			
C	-2.64429	1.024501	-0.2426	C	2.869032	-0.64485	0.748913

H	-2.47216	1.259748	-1.29346	H	3.60423	-1.04327	0.047941
H	-1.91423	1.574098	0.353085	H	2.150081	-1.4282	0.987691
H	-3.64723	1.3575	0.03304	H	3.387569	-0.34756	1.663093
C	-2.51753	-0.47263	-0.02162	C	2.164716	0.553762	0.144538
H	-2.70766	-0.74067	1.02432	H	1.403537	0.954825	0.819239
H	-3.22114	-1.02421	-0.64545	H	2.873314	1.34777	-0.0942
O	-1.22085	-0.93614	-0.40302	O	1.548143	0.205834	-1.10816
C	-0.30019	-0.95162	0.605603	C	0.212966	0.009786	-1.07067
H	-0.53768	-1.63095	1.431051	H	-0.15414	-0.23468	-2.07107
H	-0.15807	0.258079	1.094615	H	-0.43401	1.079813	-0.70796
O	0.958197	-1.18406	0.146122	O	-0.17082	-0.89813	-0.0915
C	1.559444	-0.10573	-0.58835	C	-1.4011	-0.60875	0.562414
H	1.485894	-0.31736	-1.65709	H	-1.41272	-1.2462	1.446056
C	2.980738	0.035631	-0.10369	C	-2.60512	-0.84296	-0.32511
H	3.495574	-0.92065	-0.19903	H	-2.6199	-1.88817	-0.63515
H	3.498063	0.786421	-0.70156	H	-3.51335	-0.62127	0.236139
H	2.975384	0.339927	0.942652	H	-2.58152	-0.20403	-1.20645
O	0.797322	1.070365	-0.4386	O	-1.31346	0.697906	1.077976
O	0.557108	1.284479	0.910715	O	-1.33212	1.598019	0.015958
E_{0K}=-496.6233179				E_{0K}=-496.62685			

	Structure 29				Structure 30		
C	3.296999	-0.0142	-0.4451	C	2.416971	1.21062	-0.50198
H	2.909004	0.069034	-1.46232	H	1.676831	1.814114	0.023843
H	3.653772	-1.03368	-0.28628	H	2.127607	1.124415	-1.55108
H	4.146157	0.666254	-0.35928	H	3.380295	1.72339	-0.45062
C	2.247027	0.349641	0.59177	C	2.537127	-0.17293	0.112594
H	2.67225	0.337442	1.594334	H	3.342296	-0.7355	-0.36036
H	1.828385	1.344656	0.404582	H	2.743237	-0.11512	1.187669
O	1.16907	-0.58515	0.646097	O	1.359952	-0.96643	-0.10005
C	0.420241	-0.68211	-0.49343	C	0.366533	-0.81167	0.816521
H	0.872279	-1.24701	-1.31268	H	0.625196	-1.10826	1.837111
H	0.143246	0.542522	-0.9073	H	-0.62631	-1.57679	0.359107
O	-0.83371	-1.14621	-0.24294	O	-0.2595	0.412344	0.854303
C	-1.68162	-0.25109	0.493165	C	-1.14523	0.722708	-0.23289
H	-1.70979	-0.56319	1.539122	H	-0.66613	1.460394	-0.88191
C	-3.03599	-0.26201	-0.17098	C	-2.44561	1.211884	0.35674
H	-3.40342	-1.28651	-0.23412	H	-2.25031	2.049803	1.026332
H	-3.73429	0.338058	0.412947	H	-3.11092	1.535504	-0.44427
H	-2.94756	0.152002	-1.17516	H	-2.91438	0.404141	0.918018
O	-1.10146	1.032968	0.556753	O	-1.29378	-0.39517	-1.07243
O	-0.72265	1.428267	-0.71821	O	-1.64494	-1.49322	-0.30305
E_{0K}=-496.6222447				E_{0K}=-496.6178647			

Table S45. Cartesian coordinates of the transition state 2 (TS2).

BC-eq				TBC-eq			
C	3.029715	-0.70296	0.395356	C	3.004718	0.522657	-0.60144
H	2.958735	-0.64903	1.48259	H	2.557091	0.859808	-1.53734
H	3.870172	-0.07936	0.075743	H	3.732243	-0.26216	-0.82982
H	3.227588	-1.73403	0.100997	H	3.525857	1.358521	-0.13391
C	1.756028	-0.21838	-0.2316	C	1.939462	-0.00368	0.313267
H	1.681671	-0.33071	-1.32239	H	2.264716	-0.25276	1.331473
H	0.794618	-1.00893	0.099463	H	1.082606	0.938761	0.535278
O	1.447866	1.05947	0.184847	O	1.224758	-1.02018	-0.28515
C	0.242272	1.590797	-0.30131	C	0.124709	-1.53419	0.431847
H	0.148188	1.395208	-1.37762	H	0.17808	-1.21004	1.480159
H	0.29295	2.657842	-0.09366	H	0.17488	-2.61884	0.354417
O	-0.85339	1.066223	0.394692	O	-1.08765	-1.16484	-0.14388
C	-1.69759	0.180483	-0.29566	C	-1.61521	0.091542	0.204018
H	-2.14183	0.668696	-1.17201	H	-1.66617	0.188547	1.2943
C	-2.73687	-0.30774	0.682214	C	-2.95777	0.214364	-0.47422
H	-3.30076	0.540206	1.070394	H	-3.5944	-0.61868	-0.1785
H	-3.41495	-0.99879	0.181397	H	-3.42813	1.156557	-0.19626
H	-2.23949	-0.81754	1.506314	H	-2.81507	0.18653	-1.55507
O	-0.96963	-0.87722	-0.89983	O	-0.81031	1.15923	-0.26762
O	-0.30463	-1.61058	0.064632	O	0.049805	1.59198	0.720956
E_{0K}=-496.6331929				E_{0K}=-496.6319571			

BC-ax				TBC-ax			
C	-2.39226	-0.83946	0.610257	C	2.935192	0.323367	0.529651
H	-3.24174	-0.24575	0.962147	H	3.704724	-0.44199	0.388242
H	-1.66136	-0.92977	1.415415	H	2.498766	0.194697	1.52177
H	-2.7415	-1.84376	0.368186	H	3.410397	1.304734	0.497645
C	-1.80127	-0.21013	-0.62864	C	1.90404	0.223458	-0.56938
H	-0.71803	-0.8981	-0.83473	H	1.001908	1.107399	-0.26904
H	-2.38794	-0.34782	-1.53622	H	2.263372	0.510273	-1.55696
O	-1.46314	1.128844	-0.54906	O	1.238489	-0.98201	-0.69041
C	-0.45816	1.496914	0.360023	C	0.362446	-1.37029	0.341787
H	-0.61861	1.034688	1.340257	H	0.598499	-0.84331	1.273513
H	-0.52029	2.581142	0.425197	H	0.486518	-2.44513	0.459301
O	0.808051	1.164756	-0.14176	O	-0.97303	-1.16828	-0.01022
C	1.502545	0.127132	0.497614	C	-1.56775	0.057306	0.334019
H	1.686772	0.370243	1.55143	H	-1.3751	0.283489	1.389026
C	2.778493	-0.10867	-0.27152	C	-3.03637	-0.04702	0.001543
H	3.375456	0.802994	-0.2763	H	-3.47004	-0.89316	0.533022
H	3.345104	-0.91369	0.196407	H	-3.54865	0.870884	0.286409
H	2.532468	-0.38318	-1.29631	H	-3.14871	-0.20655	-1.0714
O	0.704614	-1.04226	0.614342	O	-1.05553	1.13902	-0.42277
O	0.347166	-1.50406	-0.63877	O	0.039188	1.690987	0.213737

E_{0K}=-496.6306373	E_{0K}=-496.6288796

Table S46. Cartesian coordinates of the transition state 3 (TS3) within chair-eq1-ax2 structures.

Structure 1				Structure 2			
C	2.924707	0.224135	-0.7013	C	-2.77954	-0.51376	1.998734
H	2.520394	-0.17709	-1.63255	H	-3.30482	0.441631	2.013525
H	3.660826	-0.47659	-0.30272	H	-2.11647	-0.55691	2.86376
H	3.433924	1.159183	-0.94179	H	-3.51098	-1.31979	2.077805
C	1.836604	0.491387	0.326524	C	-1.98293	-0.65584	0.720998
H	2.247286	1.008104	1.19307	H	-1.44761	-1.6107	0.68962
H	1.04502	1.114431	-0.10252	H	-2.63692	-0.60507	-0.15899
O	1.266614	-0.69903	0.869831	O	-1.04749	0.418713	0.674041
C	0.627426	-1.50887	-0.03668	C	-0.32646	0.467689	-0.49261
H	1.277047	-1.89998	-0.82125	H	-0.95244	0.47881	-1.38857
O	-0.43111	-0.84922	-0.69569	O	0.541284	-0.63543	-0.63508
C	-1.44894	-0.43675	0.156348	C	1.508063	-0.71339	0.359367
H	-1.42157	-1.40036	1.059589	H	1.732646	0.567768	0.584614
C	-2.76091	-0.33428	-0.5601	C	2.723032	-1.45517	-0.10829
H	-3.01697	-1.28882	-1.0213	H	3.135115	-0.98397	-1.00134
H	-3.55048	-0.04831	0.135294	H	3.482661	-1.46846	0.673716
H	-2.70372	0.422773	-1.34888	H	2.463086	-2.48943	-0.35573
H	-1.15985	0.413755	0.781755	H	1.093629	-1.00384	1.329835
O	0.114853	-2.63271	0.606036	O	0.433846	1.632189	-0.54708
O	-0.73907	-2.24744	1.632537	O	1.264969	1.707461	0.564871
E_{0K}=-496.6296726				E_{0K}=-496.6285314			

Structure 3				Structure 4			
C	-1.55933	-2.01392	0.952544	C	-1.25085	2.969325	1.181721
H	-1.13675	-1.99033	1.958891	H	-0.49306	3.353244	0.50055
H	-0.80972	-2.39818	0.25997	H	-0.78002	2.773277	2.146142
H	-2.41021	-2.69873	0.956003	H	-2.02434	3.72862	1.319431
C	-2.02318	-0.62357	0.551312	C	-1.88374	1.698055	0.646535
H	-2.42712	-0.62458	-0.46826	H	-2.67883	1.3535	1.308961
H	-2.80843	-0.2756	1.222787	H	-2.31769	1.86265	-0.34663
O	-0.98771	0.353861	0.652959	O	-0.95499	0.610859	0.581106
C	-0.2375	0.524534	-0.48212	C	-0.34297	0.444695	-0.63372
H	-0.8417	0.619727	-1.38761	H	-1.04464	0.326181	-1.46362
O	0.652875	-0.54461	-0.72045	O	0.459456	-0.68824	-0.58527
C	1.611229	-0.70804	0.27195	C	1.489996	-0.60504	0.34352
H	1.808001	0.546996	0.634051	H	1.803415	0.665166	0.238252
C	2.844274	-1.37606	-0.25594	C	2.618993	-1.52472	-0.00766
H	3.255454	-0.81008	-1.09259	H	2.988646	-1.31056	-1.01109
H	3.597186	-1.45525	0.528685	H	3.434116	-1.41183	0.707506

H	2.606109	-2.38472	-0.60918	H	2.278341	-2.56465	0.018201
H	1.191664	-1.10616	1.200641	H	1.125388	-0.63215	1.373318
O	0.508318	1.69828	-0.4024	O	0.463221	1.538877	-1.02508
O	1.314652	1.669867	0.72938	O	1.400346	1.809151	-0.03366
E_{0K}=-496.6286764				E_{0K}=-496.6278814			

Structure 5				Structure 6			
C	-2.74628	1.455143	1.949877	C	-2.8412	1.936288	-0.35183
H	-2.14264	1.245597	2.834006	H	-3.47705	1.081627	-0.59233
H	-3.40842	0.607078	1.770898	H	-2.33246	2.269859	-1.25846
H	-3.35391	2.340033	2.146484	H	-3.4794	2.754643	-0.01359
C	-1.85247	1.695062	0.753964	C	-1.8538	1.579942	0.746997
H	-2.44373	1.893593	-0.14887	H	-1.15642	2.399648	0.934755
H	-1.17859	2.539453	0.917655	H	-2.37667	1.347658	1.674023
O	-1.07406	0.514124	0.554256	O	-1.10528	0.393402	0.464532
C	-0.35782	0.507469	-0.61594	C	-0.35925	0.423293	-0.68833
H	-0.98183	0.488351	-1.51355	H	-0.94843	0.381039	-1.60639
O	0.461336	-0.61525	-0.63483	O	0.498742	-0.67153	-0.69017
C	1.397186	-0.63552	0.393139	C	1.402242	-0.66965	0.365557
H	1.669852	0.648346	0.499691	H	1.635624	0.618143	0.48092
C	2.591494	-1.46372	0.030716	C	2.629301	-1.46398	0.037848
H	3.045619	-1.09711	-0.89061	H	3.100488	-1.08355	-0.86916
H	3.329607	-1.43306	0.832522	H	3.342123	-1.41477	0.861312
H	2.293133	-2.5054	-0.12462	H	2.364138	-2.51308	-0.12728
H	0.939978	-0.81722	1.368741	H	0.921291	-0.86607	1.326673
O	0.456037	1.649264	-0.78432	O	0.418105	1.593944	-0.82672
O	1.259583	1.809508	0.339252	O	1.19393	1.770854	0.314593
E_{0K}=-496.6264051				E_{0K}=-496.6252465			

Table S47. Cartesian coordinates of the transition state 3 (TS3) within chair-ax1-eq2 structures.

Structure 1				Structure 2			
C	-3.55333	-0.40831	-0.0016	C	-3.44292	0.29397	1.63742
H	-4.21767	-0.4832	-0.86425	H	-3.99599	0.90147	2.355635
H	-3.88392	0.422431	0.62298	H	-3.49048	-0.75003	1.949287
H	-3.62759	-1.33016	0.576926	H	-3.91845	0.387392	0.660631
C	-2.13116	-0.18898	-0.46471	C	-2.00622	0.758461	1.564503
H	-1.77678	-1.01688	-1.08135	H	-1.93999	1.800688	1.241688
H	-2.03282	0.740919	-1.0285	H	-1.50889	0.662478	2.537452
O	-1.31743	-0.11047	0.720857	O	-1.33486	-0.07399	0.6147
C	-0.00837	0.153969	0.533125	C	-0.01694	0.20556	0.48155
H	0.506008	0.16004	1.496341	H	0.514898	0.309769	1.438319
O	0.560818	-0.79776	-0.35247	O	0.533843	-0.80906	-0.30897
C	1.899043	-0.59598	-0.64548	C	1.874157	-0.62716	-0.61473

H	1.958173	0.739491	-0.60051	H	1.941172	0.71068	-0.66493
C	2.881836	-1.06847	0.395771	C	2.857857	-1.032	0.453817
H	2.775901	-2.14673	0.548282	H	2.747464	-2.09721	0.678197
H	3.900456	-0.86243	0.064503	H	3.876226	-0.8538	0.10607
H	2.727032	-0.56746	1.352985	H	2.709017	-0.46751	1.376015
H	2.095345	-0.91271	-1.66858	H	2.065526	-1.01475	-1.61364
O	0.144217	1.416583	-0.08729	O	0.127169	1.421257	-0.23212
O	1.493364	1.729557	-0.07128	O	1.475582	1.741559	-0.21907
E_{0K}=-496.6266108				E_{0K}=-496.6241996			

Structure 3				Structure 4			
C	-3.15011	-1.43476	1.436441	C	-2.25913	-1.71461	-1.01701
H	-3.4304	-2.35161	1.957683	H	-2.88607	-1.74333	-1.9111
H	-3.61512	-1.43672	0.450108	H	-2.77493	-2.2457	-0.21544
H	-3.52927	-0.58034	1.998024	H	-1.31847	-2.22359	-1.22816
C	-1.64641	-1.35383	1.302503	C	-2.00046	-0.27754	-0.61269
H	-1.1616	-1.33621	2.286895	H	-1.45937	0.267653	-1.38658
H	-1.24963	-2.19927	0.734314	H	-2.93112	0.25091	-0.40461
O	-1.34123	-0.14157	0.611631	O	-1.25394	-0.23819	0.62121
C	-0.01563	0.114538	0.516318	C	0.045741	0.100469	0.529307
H	0.506266	0.119859	1.483202	H	0.51951	0.019267	1.509637
O	0.586308	-0.83498	-0.35428	O	0.696702	-0.71752	-0.43412
C	1.922241	-0.5942	-0.62918	C	2.03316	-0.42259	-0.64876
H	1.944368	0.742175	-0.56803	H	2.024564	0.899933	-0.44987
C	2.910048	-1.05596	0.412608	C	3.000522	-0.96763	0.370989
H	2.833748	-2.13947	0.54614	H	2.944613	-2.0601	0.394356
H	3.925341	-0.8172	0.09324	H	4.018675	-0.67697	0.108923
H	2.734469	-0.57557	1.376859	H	2.785126	-0.58939	1.371917
H	2.136615	-0.88709	-1.65569	H	2.280248	-0.60942	-1.69264
O	0.100652	1.369932	-0.08852	O	0.161753	1.431749	0.060898
O	1.441628	1.716219	-0.03786	O	1.4928	1.800183	0.166373
E_{0K}=-496.6241072				E_{0K}=-496.6263942			

Structure 5				Structure 6			
C	-2.56126	2.101798	0.730472	C	-0.97765	-1.45265	2.710471
H	-3.1299	2.71403	1.434097	H	-1.3837	-2.34715	3.186249
H	-3.24086	1.736714	-0.04071	H	-1.16234	-0.59965	3.36646
H	-1.79761	2.719702	0.25883	H	0.100552	-1.59551	2.607615
C	-1.93256	0.930499	1.461471	C	-1.65003	-1.25166	1.362477
H	-1.2286	1.273709	2.22753	H	-1.39581	-2.05999	0.673297
H	-2.69396	0.319797	1.947848	H	-2.7327	-1.21509	1.472491
O	-1.25943	0.046337	0.556746	O	-1.32462	0.000211	0.750519
C	0.073832	0.246871	0.447278	C	-0.00295	0.222736	0.548641

H	0.597443	0.302996	1.412157	H	0.578481	0.370568	1.466657
O	0.570572	-0.78967	-0.35011	O	0.551928	-0.84479	-0.20874
C	1.926013	-0.69618	-0.62644	C	1.877225	-0.65354	-0.56465
H	2.084747	0.632455	-0.65654	H	1.903228	0.681788	-0.69026
C	2.857978	-1.18121	0.455132	C	2.89957	-0.97877	0.495114
H	2.671732	-2.23961	0.660648	H	2.823477	-2.034	0.775872
H	3.892972	-1.06717	0.130251	H	3.904323	-0.79445	0.112674
H	2.728307	-0.62115	1.382876	H	2.760097	-0.37147	1.391549
H	2.110914	-1.08369	-1.6266	H	2.051931	-1.08588	-1.54843
O	0.315101	1.462887	-0.24416	O	0.07986	1.37754	-0.23671
O	1.682697	1.688233	-0.20296	O	1.420652	1.723911	-0.29159
E_{0K}=-496.6239259				E_{0K}=-496.6217857			

Structure 7				Structure 8			
C	-2.79716	1.279614	-0.73703	C	-1.58948	0.635153	3.061176
H	-3.46934	1.21796	-1.59595	H	-2.09731	1.343125	3.719304
H	-2.09635	2.09933	-0.89658	H	-0.52574	0.654322	3.307103
H	-3.39104	1.492217	0.153206	H	-1.97286	-0.36592	3.262305
C	-2.05381	-0.03109	-0.57185	C	-1.83696	1.008558	1.610385
H	-2.74428	-0.86236	-0.42718	H	-2.90138	0.988286	1.380749
H	-1.42438	-0.25096	-1.4348	H	-1.46182	2.008639	1.375597
O	-1.24238	-0.00097	0.620252	O	-1.24933	0.055671	0.716314
C	0.078376	0.198963	0.449884	C	0.051219	0.298092	0.429429
H	0.568206	0.270111	1.423039	H	0.656532	0.613477	1.290305
O	0.63268	-0.85029	-0.33238	O	0.56095	-0.86529	-0.15779
C	1.98366	-0.72628	-0.60699	C	1.869398	-0.75229	-0.60302
H	2.094757	0.601703	-0.68454	H	1.906244	0.542083	-0.95101
C	2.923352	-1.1363	0.49872	C	2.940659	-0.9091	0.446399
H	2.769236	-2.19036	0.748258	H	2.871061	-1.89979	0.905648
H	3.956716	-1.00245	0.17623	H	3.925394	-0.80685	-0.01142
H	2.768125	-0.54173	1.400743	H	2.850748	-0.15689	1.232205
H	2.191445	-1.14396	-1.59099	H	1.990702	-1.35067	-1.50405
O	0.297464	1.392927	-0.27921	O	0.116953	1.326157	-0.54492
O	1.657604	1.656258	-0.26211	O	1.456587	1.644192	-0.70638
E_{0K}=-496.6264768				E_{0K}=-496.6235595			

Structure 9			
C	-1.13554	-2.64713	0.92506
H	-1.55902	-3.40281	1.589939
H	-0.04884	-2.66811	1.030425
H	-1.38085	-2.90375	-0.10624
C	-1.70262	-1.28268	1.274838
H	-2.78934	-1.28239	1.205711

H	-1.42686	-0.98642	2.293594
O	-1.28777	-0.26395	0.363628
C	0.030649	0.033926	0.399109
H	0.507593	-0.1711	1.367208
O	0.692889	-0.67415	-0.63868
C	2.034066	-0.36429	-0.78603
H	2.02326	0.923845	-0.42808
C	2.978628	-1.03906	0.177246
H	2.915314	-2.12584	0.0631
H	4.004299	-0.72926	-0.02717
H	2.747764	-0.78574	1.213806
H	2.30313	-0.42154	-1.83944
O	0.147674	1.401716	0.107576
O	1.478907	1.742601	0.288613
E_{0K}=-496.6222707			

Table S48. Cartesian coordinates of the transition state 3 (TS3) within chair-ax1-ax2 structures.

Structure 1				Structure 2			
C	-3.07663	0.038669	0.154398	C	-2.37445	1.355345	-1.65464
H	-2.92912	-0.38009	1.151539	H	-2.79064	0.537132	-2.24313
H	-3.40165	-0.75863	-0.51558	H	-1.60806	1.853751	-2.25036
H	-3.87462	0.780381	0.225443	H	-3.16753	2.072422	-1.43628
C	-1.81597	0.695688	-0.38461	C	-1.77816	0.828602	-0.36833
H	-2.01572	1.17202	-1.34447	H	-1.34304	1.637522	0.227761
H	-1.44099	1.46001	0.303453	H	-2.53827	0.326081	0.243438
O	-0.78085	-0.24755	-0.66194	O	-0.76174	-0.10727	-0.71669
C	-0.14745	-0.75304	0.447981	C	-0.17058	-0.70767	0.367842
H	-0.82307	-1.22052	1.166682	H	-0.89215	-1.17687	1.042046
O	0.559372	0.232422	1.172981	O	0.566116	0.196622	1.164997
C	1.676242	0.764525	0.532643	C	1.717988	0.713371	0.577628
H	2.043075	-0.262	-0.22325	H	2.054776	-0.28339	-0.22962
C	1.428002	1.900316	-0.42726	C	1.53847	1.912425	-0.31881
H	2.379994	2.269229	-0.81205	H	2.512157	2.255922	-0.67152
H	0.807895	1.578558	-1.26437	H	0.915527	1.668146	-1.17987
H	0.925931	2.723914	0.091531	H	1.069507	2.728886	0.24066
H	2.456495	0.930021	1.274494	H	2.489686	0.801092	1.341368
O	0.740063	-1.75628	0.072015	O	0.675852	-1.72916	-0.04948
O	1.667613	-1.24866	-0.82926	O	1.64593	-1.21409	-0.90069
E_{0K}=-496.622946				E_{0K}=-496.6254312			

Structure 3				Structure 4			
C	-0.53371	-1.94131	-2.50826	C	-2.28352	-0.51699	-2.43723
H	0.269691	-2.523	-2.0586	H	-1.6578	0.128288	-3.05568

H	-0.09054	-1.18522	-3.15838	H	-3.03053	0.099324	-1.93543
H	-1.15467	-2.60259	-3.11715	H	-2.79456	-1.22941	-3.08695
C	-1.39147	-1.2748	-1.44831	C	-1.43374	-1.25321	-1.42572
H	-2.22051	-0.73251	-1.90507	H	-2.04904	-1.89979	-0.78715
H	-1.81062	-2.01656	-0.75866	H	-0.67526	-1.87163	-1.91209
O	-0.66326	-0.29276	-0.7032	O	-0.78441	-0.27334	-0.61447
C	-0.14463	-0.74237	0.485329	C	-0.13384	-0.7972	0.476112
H	-0.9014	-1.17203	1.147541	H	-0.80765	-1.27781	1.19113
O	0.456574	0.311656	1.163113	O	0.540991	0.217967	1.145614
C	1.632446	0.807852	0.603613	C	1.631533	0.764049	0.469739
H	2.110175	-0.28094	0.033048	H	2.015319	-0.2697	-0.26165
C	1.484802	1.820474	-0.5019	C	1.338198	1.878762	-0.49995
H	2.471824	2.169901	-0.80911	H	2.27346	2.251995	-0.92027
H	0.96461	1.394013	-1.35803	H	0.684859	1.540374	-1.30233
H	0.909284	2.677549	-0.13842	H	0.842112	2.699691	0.027453
H	2.306049	1.083559	1.414077	H	2.420629	0.961344	1.194568
O	0.799336	-1.78274	0.335698	O	0.788914	-1.80979	0.140059
O	1.833158	-1.35608	-0.48935	O	1.680388	-1.3155	-0.80481
E_{0K}=-496.6268602				E_{0K}=-496.6288494			

Structure 5			
C	-2.30028	-2.18937	-0.74621
H	-3.05794	-1.62904	-0.19429
H	-1.79292	-2.87342	-0.06315
H	-2.80397	-2.79433	-1.5023
C	-1.32233	-1.24542	-1.42625
H	-0.5099	-1.79623	-1.90641
H	-1.82986	-0.64578	-2.18116
O	-0.76063	-0.27745	-0.53401
C	-0.08267	-0.79372	0.545406
H	-0.72804	-1.26994	1.286308
O	0.597907	0.23303	1.193351
C	1.665189	0.787707	0.489038
H	2.04432	-0.24536	-0.24099
C	1.339831	1.894089	-0.48009
H	2.2626	2.277587	-0.91842
H	0.676187	1.544791	-1.2689
H	0.842957	2.710542	0.053492
H	2.46822	0.998247	1.194696
O	0.840931	-1.79981	0.193291
O	1.711092	-1.30225	-0.77052
E_{0K}=-496.6266106			

Table S49. Cartesian coordinates of the transition state 3 (TS3) within chair-eq1-eq2

structures.

Structure 1				Structure 2			
C	-3.46314	-0.6204	-0.19588	C	-2.04717	-2.03735	-0.20778
H	-3.93739	-1.13108	-1.03576	H	-2.48782	-2.54527	-1.06864
H	-3.94754	0.346811	-0.0566	H	-2.72	-2.15197	0.643533
H	-3.6119	-1.21747	0.704857	H	-1.09386	-2.50928	0.031205
C	-1.98788	-0.4382	-0.47066	C	-1.84403	-0.56904	-0.52178
H	-1.81869	0.174041	-1.35874	H	-2.78636	-0.08188	-0.77331
H	-1.48167	-1.39689	-0.59842	H	-1.14964	-0.42627	-1.35038
O	-1.43278	0.232471	0.676355	O	-1.35478	0.12256	0.646019
C	-0.11593	0.518136	0.623108	C	-0.05568	0.475136	0.637007
H	0.195583	1.013519	1.547091	H	0.220684	0.918483	1.597577
O	0.637617	-0.661	0.404423	O	0.758963	-0.64775	0.342081
C	2.002629	-0.44882	0.368435	C	2.113142	-0.36924	0.329695
H	2.050828	0.750274	-0.20678	H	2.105668	0.868872	-0.1583
C	2.719135	-1.51128	-0.40794	C	2.880975	-1.33846	-0.51655
H	2.325728	-1.5687	-1.42362	H	2.491567	-1.34349	-1.53542
H	3.786969	-1.29527	-0.44935	H	3.937033	-1.06843	-0.53856
H	2.581326	-2.48671	0.069423	H	2.791265	-2.3508	-0.10964
H	2.414692	-0.19888	1.353439	H	2.509732	-0.17245	1.332778
O	0.151877	1.365619	-0.47871	O	0.180842	1.411925	-0.39954
O	1.457353	1.813302	-0.35815	O	1.463615	1.909163	-0.23667
E_{0K}=-496.6296726				E_{0K}=-496.6285314			

Structure 3				Structure 4			
C	-2.69644	0.685469	-1.37912	C	-3.70905	0.774247	0.88237
H	-3.18803	0.208444	-2.2301	H	-4.41128	1.571339	1.131908
H	-2.01003	1.446789	-1.75	H	-3.8068	-0.02396	1.61911
H	-3.4582	1.167389	-0.7644	H	-3.9669	0.375502	-0.09922
C	-1.94944	-0.35499	-0.56841	C	-2.29685	1.3134	0.871869
H	-1.15721	-0.82884	-1.14932	H	-2.01695	1.711021	1.855026
H	-2.62289	-1.13152	-0.20489	H	-2.1777	2.106593	0.129435
O	-1.38511	0.240669	0.617907	O	-1.42611	0.226234	0.545324
C	-0.06738	0.516019	0.589314	C	-0.11446	0.559936	0.54792
H	0.228317	1.027458	1.509514	H	0.208182	1.117723	1.441163
O	0.680982	-0.67542	0.41286	O	0.610461	-0.62513	0.405051
C	2.048193	-0.47819	0.400527	C	1.978903	-0.42095	0.375774
H	2.122181	0.701824	-0.20452	H	2.048121	0.753712	-0.25127
C	2.769928	-1.56875	-0.33105	C	2.692104	-1.52288	-0.34537
H	2.398322	-1.65032	-1.35329	H	2.305731	-1.62161	-1.36031
H	3.840702	-1.36501	-0.35493	H	3.762403	-1.31924	-0.38518
H	2.610828	-2.52911	0.169534	H	2.538334	-2.47442	0.173389
H	2.442357	-0.20639	1.387145	H	2.381723	-0.13126	1.353743

O	0.234594	1.334401	-0.5273	O	0.163261	1.357855	-0.59071
O	1.543925	1.769045	-0.39671	O	1.465777	1.814692	-0.46267
E_{0K}=-496.6286764				E_{0K}=-496.6278814			

Structure 5				Structure 6			
C	3.191559	0.235383	0.645081	C	-2.02018	2.128972	2.099841
H	4.200756	0.49196	0.315015	H	-2.83686	2.840446	2.23475
H	3.264803	-0.36365	1.55376	H	-1.09171	2.701019	2.051442
H	2.648835	1.152309	0.873312	H	-1.99035	1.471714	2.971374
C	2.482608	-0.55456	-0.4386	C	-2.2615	1.328408	0.830949
H	3.032069	-1.46465	-0.6818	H	-2.19047	1.965464	-0.05345
H	2.376869	0.036812	-1.35454	H	-3.2474	0.866622	0.848338
O	1.189966	-0.99616	-0.00386	O	-1.36895	0.216942	0.678789
C	0.158244	-0.21857	-0.40378	C	-0.05081	0.529544	0.660488
H	0.140035	-0.01048	-1.48491	H	0.326313	1.004018	1.577466
O	-1.01418	-0.85738	0.004441	O	0.638935	-0.65846	0.403793
C	-2.1583	-0.15958	-0.34002	C	2.009978	-0.47962	0.364535
H	-1.73692	1.097266	-0.21646	H	2.090991	0.735361	-0.17667
C	-3.30704	-0.49258	0.561465	C	2.688056	-1.53902	-0.44848
H	-3.04355	-0.28831	1.59972	H	2.280966	-1.55689	-1.45993
H	-4.18457	0.094629	0.289987	H	3.761196	-1.35248	-0.49496
H	-3.5586	-1.55432	0.474864	H	2.525376	-2.52268	0.003234
H	-2.35624	-0.1824	-1.4184	H	2.436581	-0.26934	1.352754
O	0.211152	1.027742	0.275088	O	0.211007	1.405036	-0.42337
O	-0.76018	1.842073	-0.28759	O	1.526608	1.823751	-0.3
E_{0K}=-496.6264051				E_{0K}=-496.6252465			

Structure 7				Structure 8			
C	-3.36387	-0.78808	1.60036	C	-1.48482	-0.05177	3.095944
H	-3.73895	-1.3917	2.428494	H	-1.95391	-0.69434	3.843295
H	-3.61998	-1.28231	0.662686	H	-1.85553	0.96565	3.234667
H	-3.85309	0.186207	1.624971	H	-0.40854	-0.06514	3.280606
C	-1.86463	-0.62895	1.712442	C	-1.82819	-0.56369	1.706939
H	-1.35675	-1.59649	1.679702	H	-2.90691	-0.64264	1.581522
H	-1.58908	-0.12096	2.645256	H	-1.3839	-1.54543	1.528049
O	-1.43306	0.164306	0.605676	O	-1.42629	0.327352	0.662304
C	-0.11617	0.474236	0.634958	C	-0.10105	0.604843	0.607008
H	0.211703	0.961457	1.566026	H	0.28297	1.197845	1.448646
O	0.654537	-0.69675	0.418654	O	0.641623	-0.59869	0.501623
C	2.014575	-0.45296	0.377165	C	2.002218	-0.3825	0.379483
H	2.030272	0.751541	-0.18902	H	2.009498	0.750068	-0.32493
C	2.748789	-1.4909	-0.41544	C	2.69285	-1.51681	-0.31378
H	2.342796	-1.55053	-1.42577	H	2.247802	-1.68602	-1.29485

H	3.810419	-1.24822	-0.46765	H	3.7544	-1.29874	-0.43307
H	2.640692	-2.47326	0.055454	H	2.591991	-2.43656	0.271392
H	2.430486	-0.19986	1.360071	H	2.458763	-0.02334	1.30993
O	0.113115	1.326455	-0.45105	O	0.093002	1.314974	-0.58419
O	1.408391	1.803944	-0.32465	O	1.396082	1.786474	-0.56369
E_{0K}=-496.6266108				E_{0K}=-496.6241996			

Structure 9			
C	-1.56115	-1.96895	1.867543
H	-2.16831	-2.38811	2.672613
H	-0.51746	-1.97315	2.187385
H	-1.64923	-2.60776	0.987865
C	-2.04005	-0.56468	1.545295
H	-1.9192	0.104384	2.405163
H	-3.09225	-0.56694	1.264727
O	-1.37271	0.000742	0.41605
C	-0.06524	0.288925	0.603224
H	0.203845	0.511294	1.646977
O	0.72655	-0.78261	0.120495
C	2.085689	-0.55036	0.212752
H	2.126651	0.759141	-0.01453
C	2.86287	-1.35426	-0.78471
H	2.508877	-1.14505	-1.79468
H	3.925071	-1.1173	-0.71901
H	2.733516	-2.42402	-0.59162
H	2.450113	-0.56812	1.247604
O	0.221816	1.404879	-0.19938
O	1.509391	1.814024	0.110601
E_{0K}=-496.6246415			

Table S50. Cartesian coordinates of the transition state 3 (TS3) within boat-eq1 structures.

Structure 1				Structure 2			
C	-3.34301	-0.33988	-0.40363	C	-3.04654	-1.54567	1.374013
H	-3.00047	-0.06978	-1.40439	H	-3.61053	-0.68231	1.72874
H	-3.78283	0.543831	0.06009	H	-2.50002	-1.97292	2.215505
H	-4.11786	-1.10202	-0.5096	H	-3.74699	-2.29237	0.996236
C	-2.20967	-0.87123	0.456434	C	-2.0869	-1.13371	0.280528
H	-2.57272	-1.14154	1.44743	H	-1.50171	-1.98599	-0.07771
H	-1.74488	-1.75887	0.016247	H	-2.62336	-0.6981	-0.57123
O	-1.20903	0.124575	0.688942	O	-1.20465	-0.15363	0.827059
C	-0.28308	0.224261	-0.3098	C	-0.29744	0.326029	-0.07314
H	-0.71173	0.173532	-1.31585	H	-0.74754	0.599859	-1.03411
O	0.672631	-0.82311	-0.26148	O	0.707662	-0.62513	-0.38632

C	1.873213	-0.49375	0.343012	C	1.913814	-0.44582	0.26887
H	2.123012	0.630669	-0.28327	H	2.082942	0.837621	0.059145
C	2.911907	-1.54612	0.1121	C	2.993734	-1.29313	-0.32733
H	3.02712	-1.73911	-0.95529	H	3.075857	-1.10614	-1.39883
H	3.869458	-1.23002	0.526231	H	3.950042	-1.07879	0.150024
H	2.615703	-2.48106	0.598069	H	2.764158	-2.35353	-0.18273
H	1.754577	-0.11948	1.365654	H	1.81809	-0.44693	1.360097
O	0.327272	1.465164	-0.0731	O	0.256867	1.440094	0.573511
O	1.477177	1.550302	-0.83862	O	1.373875	1.851553	-0.13266
E_{0K}=-496.621214				E_{0K}=-496.6232201			

Structure 3				Structure 4			
C	-1.87811	-2.12477	-0.5996	C	-1.75809	2.059973	2.389066
H	-1.40093	-2.78879	0.122755	H	-0.93317	2.714069	2.108117
H	-1.18067	-1.96038	-1.42263	H	-1.49579	1.546553	3.315265
H	-2.76981	-2.61677	-0.99392	H	-2.64763	2.667948	2.569355
C	-2.26958	-0.81795	0.06794	C	-2.04581	1.044275	1.298225
H	-2.72017	-0.12575	-0.65298	H	-2.89155	0.412052	1.570454
H	-2.99069	-0.9881	0.866399	H	-2.28305	1.539233	0.349504
O	-1.17052	-0.17128	0.70975	O	-0.95279	0.141535	1.098552
C	-0.23145	0.345309	-0.13409	C	-0.06346	0.505818	0.131572
H	-0.64369	0.643872	-1.10453	H	-0.54708	0.833203	-0.7964
O	0.804453	-0.57673	-0.43005	O	0.744624	-0.59431	-0.18589
C	1.970555	-0.41246	0.296943	C	2.057852	-0.52891	0.248492
H	2.139961	0.876934	0.139954	H	2.35263	0.702635	-0.08872
C	3.088603	-1.23218	-0.26708	C	2.906469	-1.55461	-0.43466
H	3.228859	-1.00729	-1.32521	H	2.831724	-1.45099	-1.51791
H	4.015122	-1.02862	0.270014	H	3.948105	-1.44544	-0.13243
H	2.859565	-2.29824	-0.17196	H	2.569357	-2.56006	-0.16428
H	1.814446	-0.45387	1.380387	H	2.148851	-0.44751	1.336765
O	0.281514	1.449266	0.568442	O	0.725364	1.562098	0.651954
O	1.431624	1.890421	-0.06293	O	1.768219	1.803636	-0.22878
E_{0K}=-496.6217755				E_{0K}=-496.6226629			

Structure 5				Structure 6			
C	-3.31748	0.560485	1.820139	C	-2.7096	1.954667	0.020107
H	-2.93769	0.282981	2.804089	H	-3.14315	1.177592	-0.61237
H	-3.69973	-0.33527	1.329224	H	-2.05414	2.581634	-0.58672
H	-4.13795	1.268232	1.949803	H	-3.51774	2.588749	0.389563
C	-2.21774	1.187158	0.993011	C	-1.98128	1.334934	1.202142
H	-2.58109	1.462808	-0.00475	H	-1.45482	2.095162	1.784257
H	-1.81854	2.083571	1.47462	H	-2.68518	0.825686	1.858895
O	-1.17595	0.217003	0.855553	O	-1.05958	0.304525	0.824012

C	-0.17586	0.597699	0.00837	C	-0.02518	0.70439	0.025499
H	-0.54642	0.962873	-0.95719	H	-0.34164	1.165582	-0.91486
O	0.651925	-0.50189	-0.25104	O	0.741038	-0.41903	-0.31355
C	1.901231	-0.47302	0.346272	C	1.960359	-0.5292	0.332059
H	2.248272	0.767767	0.095381	H	2.401501	0.699076	0.195292
C	2.817803	-1.48535	-0.26504	C	2.830505	-1.55504	-0.32316
H	2.880467	-1.33999	-1.34426	H	2.949367	-1.33212	-1.38426
H	3.814476	-1.40343	0.168766	H	3.810901	-1.57884	0.152754
H	2.439139	-2.49507	-0.07849	H	2.375213	-2.54602	-0.23185
H	1.855939	-0.43259	1.439652	H	1.86973	-0.57052	1.422692
O	0.551408	1.623361	0.659018	O	0.74645	1.625648	0.774838
O	1.698119	1.880091	-0.07418	O	1.931864	1.859418	0.098153
E_{0K}=-496.6239521				E_{0K}=-496.6209523			

Structure 7				Structure 8			
C	-0.97791	-2.17936	1.983876	C	-1.94857	-0.53488	3.07094
H	-0.21529	-2.60963	1.334178	H	-2.56013	-1.3215	2.627231
H	-1.95724	-2.51896	1.643354	H	-2.54493	0.375998	3.133664
H	-0.82202	-2.53856	3.003685	H	-1.66567	-0.83832	4.080359
C	-0.91112	-0.66515	1.949529	C	-0.71104	-0.29685	2.234986
H	-1.66646	-0.22076	2.598223	H	-0.09543	0.502101	2.656038
H	0.06407	-0.29531	2.273008	H	-0.10996	-1.20706	2.152842
O	-1.20398	-0.1823	0.627511	O	-1.15546	0.083742	0.925509
C	-0.14941	0.243838	-0.10577	C	-0.18088	0.357953	0.021002
H	-0.48348	0.448658	-1.12274	H	-0.64288	0.534438	-0.95003
O	0.883452	-0.74161	-0.17954	O	0.733123	-0.72242	-0.13969
C	2.157715	-0.37893	0.224566	C	2.052655	-0.49468	0.210769
H	2.185573	0.888353	-0.1113	H	2.212946	0.731712	-0.22194
C	3.21032	-1.18509	-0.47229	C	2.973167	-1.4743	-0.44865
H	3.108732	-1.08882	-1.55408	H	2.843434	-1.4473	-1.53132
H	4.204201	-0.85264	-0.17142	H	4.010155	-1.24415	-0.20312
H	3.106185	-2.24383	-0.21455	H	2.751981	-2.48979	-0.10533
H	2.256504	-0.28128	1.312259	H	2.195259	-0.32814	1.285333
O	0.36709	1.415454	0.483987	O	0.515309	1.504878	0.457797
O	1.429316	1.850167	-0.29179	O	1.544166	1.757833	-0.43341
E_{0K}=-496.6234072				E_{0K}=-496.6250541			

Table S51. Cartesian coordinates of the transition state 3 (TS3) within boat-ax1 structures.

Structure 1				Structure 2			
C	3.305126	0.220239	0.096054	C	2.877772	-1.85547	-0.85221
H	3.030966	1.066919	0.728298	H	3.274774	-1.24502	-1.66406
H	3.558678	0.598303	-0.89502	H	2.246208	-2.63471	-1.28048
H	4.191286	-0.24802	0.529515	H	3.710165	-2.32852	-0.32854

C	2.1807	-0.79562	-0.00456	C	2.079131	-1.00155	0.106567
H	2.475196	-1.63465	-0.63411	H	1.660874	-1.60156	0.920368
H	1.901519	-1.194	0.975713	H	2.701159	-0.21038	0.5426
O	1.023826	-0.24454	-0.64101	O	1.013902	-0.4039	-0.63215
C	0.200503	0.444406	0.204367	C	0.213544	0.405356	0.123214
H	0.734925	1.085892	0.912482	H	0.779188	1.102254	0.752133
O	-0.5892	-0.41634	1.011015	O	-0.60802	-0.32612	1.020241
C	-1.90214	-0.60357	0.606764	C	-1.93353	-0.49045	0.647265
H	-2.21906	0.653279	0.356144	H	-2.19094	0.743362	0.252574
C	-2.11586	-1.38412	-0.66183	C	-2.19887	-1.40084	-0.52102
H	-1.68908	-2.38629	-0.54933	H	-1.82054	-2.40343	-0.29509
H	-3.18299	-1.47757	-0.86705	H	-3.27135	-1.46464	-0.70896
H	-1.62548	-0.901	-1.50809	H	-1.69478	-1.04331	-1.42005
H	-2.48812	-0.90631	1.472921	H	-2.52472	-0.66057	1.545484
O	-0.60367	1.19968	-0.66294	O	-0.56099	1.085197	-0.82874
O	-1.66972	1.720016	0.04885	O	-1.59559	1.736971	-0.18178
E_{0K}=-496.6204918				E_{0K}=-496.6225597			

Structure 3				Structure 4			
C	2.06279	-1.53383	1.361058	C	1.172034	1.208235	-2.96419
H	1.541694	-2.45588	1.098408	H	0.55662	2.031235	-2.59877
H	1.491005	-1.03157	2.142927	H	0.564003	0.602122	-3.63731
H	3.047522	-1.78792	1.759128	H	2.010996	1.624241	-3.52634
C	2.219871	-0.65325	0.13369	C	1.697759	0.355785	-1.82296
H	2.709488	0.294366	0.387019	H	2.345033	-0.43714	-2.19576
H	2.820653	-1.14877	-0.62797	H	2.27513	0.958482	-1.112
O	0.977104	-0.37788	-0.51257	O	0.664933	-0.3329	-1.11345
C	0.142108	0.459298	0.170184	C	-0.11682	0.447328	-0.31438
H	0.678964	1.179689	0.797706	H	0.415587	1.319411	0.08469
O	-0.73275	-0.22708	1.050103	O	-0.56466	-0.30443	0.785889
C	-2.02656	-0.4356	0.59724	C	-1.91411	-0.6215	0.835821
H	-2.27735	0.774827	0.135556	H	-2.4311	0.519209	0.419532
C	-2.19403	-1.40253	-0.54342	C	-2.38088	-1.6945	-0.10891
H	-1.81155	-2.38491	-0.24701	H	-1.83358	-2.62042	0.095295
H	-3.2497	-1.49869	-0.80004	H	-3.44756	-1.87733	0.027094
H	-1.63644	-1.07438	-1.42187	H	-2.19105	-1.4106	-1.14508
H	-2.67284	-0.58009	1.461318	H	-2.2018	-0.72955	1.880289
O	-0.58322	1.105269	-0.84752	O	-1.21492	0.87555	-1.09923
O	-1.66585	1.762894	-0.2916	O	-2.13436	1.499699	-0.27167
E_{0K}=-496.6211073				E_{0K}=-496.6219042			

Structure 5				Structure 6			
C	2.848393	-0.09853	-2.27775	C	2.628454	1.84081	-0.67575

H	2.344151	-0.77486	-2.96894	H	3.299183	1.017578	-0.42668
H	3.412771	-0.6932	-1.5585	H	2.058871	2.10607	0.21723
H	3.544205	0.523237	-2.84353	H	3.228816	2.70793	-0.95843
C	1.837333	0.770809	-1.56485	C	1.718783	1.445559	-1.82539
H	2.328976	1.451482	-0.85901	H	1.030448	2.250406	-2.09786
H	1.256243	1.368061	-2.27265	H	2.300342	1.188521	-2.70961
O	0.959873	-0.09482	-0.83938	O	0.971523	0.261476	-1.52016
C	0.067561	0.56467	-0.04431	C	-0.17921	0.493672	-0.84666
H	0.532997	1.353299	0.559553	H	-0.10004	1.235964	-0.03818
O	-0.52497	-0.34637	0.841079	O	-0.62239	-0.73587	-0.35433
C	-1.86703	-0.63957	0.644953	C	-1.81898	-0.64458	0.33506
H	-2.32217	0.566973	0.350069	H	-2.43195	0.326375	-0.34328
C	-2.19065	-1.5338	-0.51999	C	-2.56842	-1.94124	0.325853
H	-1.67331	-2.49072	-0.39648	H	-1.9854	-2.71755	0.831469
H	-3.26499	-1.71645	-0.56607	H	-3.52175	-1.83184	0.843364
H	-1.85827	-1.08791	-1.45848	H	-2.74973	-2.26472	-0.69963
H	-2.30117	-0.91079	1.605737	H	-1.70739	-0.14779	1.306357
O	-0.90345	1.136089	-0.90156	O	-1.15947	0.953086	-1.76375
O	-1.9352	1.638238	-0.12659	O	-2.26495	1.336977	-1.02033
E_{0K}=-496.6233116				E_{0K}=-496.6259924			

Table S52 . Cartesian coordinates of the transition state 4 (TS4) within chair-eq1 structures.

	Structure 1				Structure 2		
C	2.836701	-0.24147	-0.93947	C	-3.29778	-1.33816	-0.72014
H	2.34895	-1.21621	-0.94516	H	-3.84622	-0.97518	0.150337
H	3.655877	-0.26217	-0.21878	H	-3.19014	-2.42029	-0.63677
H	3.252098	-0.04493	-1.93064	H	-3.87711	-1.11137	-1.61697
C	1.842132	0.840677	-0.56878	C	-1.94055	-0.67637	-0.79963
H	2.310657	1.825555	-0.57005	H	-1.36718	-1.04652	-1.65306
H	0.997506	0.861442	-1.25906	H	-2.02779	0.409158	-0.87648
O	1.367562	0.641972	0.776107	O	-1.24709	-1.00399	0.41544
C	0.109472	0.157104	0.902859	C	0.045906	-0.59924	0.490187
H	-0.10978	-0.02564	1.95916	H	0.450019	-0.84891	1.476125
O	-0.02626	-1.00643	0.143791	O	0.127007	0.768644	0.237983
C	-1.20771	-1.76907	0.354209	C	1.371094	1.392441	0.526295
H	-0.99392	-2.75939	-0.05789	H	1.156687	2.46372	0.576968
C	-2.40646	-1.1552	-0.31444	C	2.408127	1.100451	-0.52288
H	-2.26679	-0.87807	-1.35765	H	2.087725	1.260378	-1.55063
H	-3.36509	-1.61421	-0.08283	H	3.418378	1.434154	-0.29625
H	-2.45872	0.056609	0.290656	H	2.479035	-0.25164	-0.4632
H	-1.38776	-1.88619	1.430352	H	1.726532	1.075094	1.514934
O	-0.79198	1.16925	0.438883	O	0.789671	-1.33942	-0.48415
O	-2.05221	0.917673	0.955011	O	2.129904	-1.31099	-0.1371
E_{0K}=-496.6187812				E_{0K}=-496.6200937			

Structure 3				Structure 4			
C	-1.60076	-0.4806	-1.97477	C	-1.9799	-0.56601	2.781955
H	-1.52065	-1.55629	-2.13774	H	-0.99423	-0.1999	3.078171
H	-0.63323	-0.02678	-2.18983	H	-1.99567	-1.65386	2.873577
H	-2.33923	-0.07228	-2.66879	H	-2.70917	-0.15042	3.479892
C	-2.0403	-0.18749	-0.55173	C	-2.33394	-0.14011	1.366568
H	-2.05315	0.886297	-0.35648	H	-3.35417	-0.43227	1.12118
H	-3.03674	-0.5867	-0.36537	H	-2.24215	0.941467	1.249408
O	-1.23581	-0.83427	0.446074	O	-1.54192	-0.79118	0.372091
C	0.07675	-0.49426	0.530614	C	-0.19465	-0.60499	0.47197
H	0.469718	-0.79209	1.508149	H	0.273708	-1.12626	1.31972
O	0.234546	0.870879	0.313738	O	0.077302	0.761646	0.546933
C	1.508121	1.417641	0.632343	C	1.425559	1.107007	0.834087
H	1.352913	2.498044	0.70105	H	1.403061	2.156839	1.139841
C	2.542477	1.086666	-0.4075	C	2.321123	0.913462	-0.359
H	2.245492	1.279856	-1.43674	H	1.961166	1.359667	-1.2841
H	3.56533	1.363948	-0.16241	H	3.387148	1.026615	-0.17436
H	2.540873	-0.27122	-0.37156	H	2.162766	-0.40625	-0.62035
H	1.828634	1.061247	1.61934	H	1.789369	0.516969	1.685771
O	0.791979	-1.25255	-0.45592	O	0.310898	-1.18021	-0.71813
O	2.124548	-1.3133	-0.08034	O	1.656531	-1.45093	-0.52959
E_{0K}=-496.6182268				E_{0K}=-496.6162763			

Structure 5				Structure 6			
C	-3.61764	0.156008	1.288824	C	-1.82962	1.255291	2.389489
H	-3.82767	-0.91172	1.360485	H	-2.14255	2.009131	1.666066
H	-3.96317	0.512916	0.317904	H	-0.7889	1.450496	2.652969
H	-4.17205	0.677789	2.070833	H	-2.43731	1.353707	3.291722
C	-2.13556	0.41622	1.440571	C	-2.00946	-0.13631	1.807001
H	-1.90696	1.482079	1.369057	H	-1.63844	-0.90397	2.496948
H	-1.76672	0.047127	2.406715	H	-3.06202	-0.33945	1.613517
O	-1.46914	-0.28157	0.390464	O	-1.37784	-0.30421	0.53998
C	-0.11094	-0.26183	0.485504	C	-0.01819	-0.27015	0.560824
H	0.273937	-0.71063	1.415258	H	0.420403	-0.6346	1.503202
O	0.334076	1.056285	0.37521	O	0.398761	1.036273	0.305852
C	1.716159	1.270089	0.627553	C	1.789328	1.293093	0.448529
H	1.823755	2.34664	0.78738	H	1.880749	2.380633	0.521021
C	2.573765	0.808413	-0.51881	C	2.581217	0.762864	-0.71478
H	2.263707	1.162125	-1.50024	H	2.19603	1.030676	-1.69675
H	3.646999	0.81568	-0.34135	H	3.663421	0.80568	-0.61303
H	2.254137	-0.50402	-0.59325	H	2.289867	-0.55658	-0.65693
H	2.011219	0.761991	1.554949	H	2.157363	0.862261	1.389411

O	0.320742	-1.05849	-0.60034	O	0.377285	-1.15942	-0.47229
O	1.624938	-1.45572	-0.35387	O	1.708179	-1.49114	-0.27639
E_{0K}=-496.6181978				E_{0K}=-496.6151296			

Structure 7				Structure 8			
C	-2.21096	-2.75154	-0.39177	C	-3.03421	-2.14718	1.628767
H	-1.36529	-2.86161	-1.07018	H	-3.61094	-1.84735	0.753117
H	-3.00203	-2.20075	-0.9027	H	-3.27569	-1.47274	2.451182
H	-2.58993	-3.74211	-0.12988	H	-3.3243	-3.16143	1.908307
C	-1.79173	-2.00934	0.862706	C	-1.55464	-2.09687	1.3202
H	-2.62892	-1.90992	1.555649	H	-0.95874	-2.38664	2.194923
H	-0.98121	-2.53597	1.376923	H	-1.29737	-2.76134	0.491782
O	-1.38021	-0.67235	0.556461	O	-1.23782	-0.75006	0.966877
C	-0.03591	-0.46934	0.563349	C	0.083998	-0.53666	0.726562
H	0.461406	-0.78691	1.493741	H	0.750336	-0.94969	1.501156
O	0.150658	0.874454	0.325392	O	0.237612	0.827263	0.601579
C	1.478448	1.350501	0.498582	C	1.57953	1.291443	0.544826
H	1.390792	2.439386	0.545073	H	1.519912	2.368589	0.723168
C	2.386934	0.936649	-0.62711	C	2.231218	1.006434	-0.78103
H	1.99732	1.120692	-1.62666	H	1.646292	1.289667	-1.65416
H	3.4405	1.17162	-0.49164	H	3.292954	1.235695	-0.84183
H	2.329918	-0.40903	-0.56721	H	2.1699	-0.34001	-0.85134
H	1.877872	1.005313	1.460898	H	2.163661	0.84873	1.361989
O	0.523465	-1.27898	-0.48309	O	0.405513	-1.22106	-0.49151
O	1.879618	-1.43898	-0.24387	O	1.778558	-1.39958	-0.55262
E_{0K}=-496.6178425				E_{0K}=-496.6193951			

Structure 9			
C	-0.83782	-2.96438	1.807377
H	-0.89203	-2.47676	2.783173
H	0.210289	-3.10888	1.537593
H	-1.29481	-3.95202	1.892305
C	-1.58521	-2.15682	0.75876
H	-1.44805	-2.59016	-0.23415
H	-2.6509	-2.13049	0.982287
O	-1.21096	-0.77568	0.725811
C	0.115856	-0.52621	0.547315
H	0.767663	-0.93195	1.334576
O	0.233606	0.845434	0.467766
C	1.563405	1.343412	0.511836
H	1.465075	2.415091	0.705356
C	2.309659	1.101973	-0.77265
H	1.780385	1.398376	-1.67648

H	3.368454	1.351502	-0.7552
H	2.280188	-0.24165	-0.88704
H	2.102626	0.898864	1.358331
O	0.513296	-1.16494	-0.67332
O	1.889891	-1.32182	-0.6617
E_{0K}=-496.616992			

Table S53. Cartesian coordinates of the transition state 4 (TS4) within twist-chair structures.

Structure 1				Structure 2			
C	2.766505	0.958433	-0.08679	C	3.469987	-1.09757	-0.59081
H	2.065939	1.614496	0.429986	H	3.393914	-0.48381	-1.4893
H	2.756833	1.196317	-1.15205	H	3.40671	-2.14674	-0.88164
H	3.770919	1.146803	0.299165	H	4.44167	-0.91908	-0.12709
C	2.397176	-0.50037	0.120804	C	2.360123	-0.7516	0.376742
H	3.132227	-1.15379	-0.35065	H	2.424882	-1.36423	1.284523
H	2.358012	-0.74744	1.187567	H	2.401184	0.301776	0.670394
O	1.150094	-0.82725	-0.4935	O	1.119979	-1.01331	-0.27558
C	0.061116	-0.74125	0.340663	C	0.023733	-0.7445	0.509811
H	0.173696	-1.33281	1.25492	H	0.08802	-1.19681	1.505
O	-0.22277	0.553584	0.760091	O	-0.18039	0.61457	0.718718
C	-0.82054	1.374589	-0.24751	C	-0.73431	1.302725	-0.40612
H	-0.47186	2.394738	-0.06074	H	-0.33073	2.318686	-0.37399
C	-2.3206	1.287461	-0.13288	C	-2.23675	1.317137	-0.29107
H	-2.89461	1.565259	-1.01383	H	-2.79447	1.499577	-1.20679
H	-2.4803	-0.04568	0.010286	H	-2.47226	0.030468	0.038655
H	-2.73112	1.645406	0.809355	H	-2.62525	1.828327	0.587729
H	-0.47124	1.070598	-1.23719	H	-0.40442	0.833274	-1.33576
O	-0.97026	-1.265	-0.47951	O	-1.02579	-1.32568	-0.24447
O	-2.17088	-1.16472	0.1951	O	-2.22586	-1.06534	0.387922
E_{0K}=-496.6187711				E_{0K}=-496.6207275			

Structure 3				Structure 4			
C	2.820888	-1.30013	1.505654	C	0.526109	-0.59586	-2.93397
H	2.955588	-2.25591	0.997797	H	-0.54628	-0.44522	-2.80715
H	2.130733	-1.44651	2.338687	H	0.69659	-1.65958	-3.10591
H	3.781311	-0.98463	1.918714	H	0.857868	-0.04265	-3.81588
C	2.310045	-0.25601	0.5272	C	1.314693	-0.13555	-1.71846
H	2.155805	0.713113	1.011796	H	2.382227	-0.27233	-1.89155
H	3.020152	-0.11447	-0.28735	H	1.153105	0.922939	-1.49688
O	1.097141	-0.66941	-0.10439	O	1.048772	-0.91471	-0.5509
C	-0.03263	-0.40327	0.634249	C	-0.05602	-0.62342	0.202171
H	0.054955	-0.68235	1.688269	H	0.040173	-1.15453	1.148269
O	-0.38189	0.942225	0.626155	O	-0.20306	0.737295	0.488693

C	-0.97059	1.384835	-0.59987	C	-1.14786	1.485334	-0.27622
H	-0.67335	2.429829	-0.72453	H	-0.80465	2.523335	-0.22306
C	-2.46952	1.2594	-0.50519	C	-2.5276	1.347029	0.304689
H	-3.01708	1.231353	-1.44449	H	-3.35153	1.682861	-0.32098
H	-2.58225	0.026449	0.028414	H	-2.63205	0.000967	0.361405
H	-2.93293	1.862741	0.273154	H	-2.612	1.613806	1.356226
H	-0.56829	0.812941	-1.4391	H	-1.13865	1.183354	-1.32644
O	-1.00223	-1.20425	-0.01946	O	-1.19766	-1.1186	-0.49712
O	-2.23653	-0.9684	0.553889	O	-2.27619	-1.11292	0.371438
E_{0K}=-496.6188506				E_{0K}=-496.6163149			

Structure 5				Structure 6			
C	2.691678	-0.2193	-2.37493	C	2.743913	-2.56979	-0.59747
H	3.488156	-0.23903	-1.62995	H	3.221015	-2.37553	0.363898
H	2.949245	0.510066	-3.14491	H	3.08874	-1.82298	-1.31382
H	2.621754	-1.20554	-2.83501	H	3.049689	-3.55665	-0.94915
C	1.376958	0.15066	-1.72425	C	1.23873	-2.50895	-0.46195
H	1.439479	1.135642	-1.25109	H	0.744235	-2.69637	-1.41842
H	0.565628	0.156197	-2.45913	H	0.878568	-3.25001	0.262709
O	1.11253	-0.83391	-0.72333	O	0.899037	-1.20196	0.003998
C	-0.05564	-0.70987	-0.02365	C	-0.42242	-1.04946	0.346675
H	-0.04474	-1.44647	0.77845	H	-0.78423	-1.83428	1.019827
O	-0.23478	0.550336	0.557858	O	-0.6171	0.157916	0.972089
C	-1.08516	1.481938	-0.11005	C	-0.70035	1.281894	0.091248
H	-0.74639	2.469446	0.218421	H	-0.29426	2.131404	0.646789
C	-2.52135	1.253133	0.271593	C	-2.14242	1.519476	-0.2771
H	-3.26989	1.747462	-0.34361	H	-2.32544	2.119943	-1.16541
H	-2.63334	-0.0653	0.001619	H	-2.53847	0.268179	-0.5854
H	-2.72155	1.272081	1.340995	H	-2.79888	1.740115	0.562643
H	-0.96132	1.429362	-1.19412	H	-0.07599	1.121491	-0.78967
O	-1.1153	-1.00509	-0.92966	O	-1.13603	-1.12007	-0.89427
O	-2.28356	-1.16291	-0.20521	O	-2.48088	-0.90724	-0.65917
E_{0K}=-496.6184807				E_{0K}=-496.621793			

Structure 7			
C	0.418116	-3.07326	-1.79089
H	0.535734	-2.59881	-2.76651
H	-0.63851	-3.07228	-1.52431
H	0.765215	-4.10645	-1.86499
C	1.233407	-2.3276	-0.75078
H	1.110319	-2.77817	0.24007
H	2.295057	-2.34701	-1.00277
O	0.872274	-0.94369	-0.69297

C	0.057393	-0.59109	0.35424
H	0.432778	-0.9292	1.325716
O	-0.07783	0.773817	0.412859
C	-1.01238	1.323128	-0.5202
H	-0.63683	2.318045	-0.77371
C	-2.36996	1.409677	0.12894
H	-3.22378	1.501501	-0.5387
H	-2.46615	0.188845	0.689953
H	-2.41498	2.043817	1.012499
H	-1.03426	0.724616	-1.43285
O	-1.19853	-1.23253	0.085913
O	-2.10976	-0.87307	1.061885
E_{0K}=-496.6204349			

Table S54. Cartesian coordinates of the transition state 4 (TS4) within chair-ax structures.

Structure 1				Structure 2			
C	-3.16186	-0.45295	-0.70314	C	-2.10595	1.662539	-0.68069
H	-2.81575	-0.6156	-1.72486	H	-1.3836	2.389392	-0.31236
H	-3.38008	-1.42134	-0.25113	H	-1.87071	1.438823	-1.72226
H	-4.08133	0.133947	-0.7379	H	-3.10474	2.103477	-0.63592
C	-2.10669	0.28121	0.09399	C	-2.08521	0.386019	0.141403
H	-1.87688	1.254125	-0.34737	H	-2.24046	0.601943	1.204932
H	-2.43334	0.44101	1.129344	H	-2.87775	-0.2896	-0.18351
O	-0.92908	-0.52391	0.093943	O	-0.87587	-0.35961	-0.01659
C	0.046946	-0.10489	0.964724	C	0.096327	-0.11305	0.920279
H	-0.2797	-0.10455	2.009991	H	-0.27399	-0.17766	1.948576
O	1.130381	-0.94895	0.886772	O	1.103522	-1.04288	0.804333
C	1.713766	-1.14966	-0.4029	C	1.735357	-1.17902	-0.4708
H	2.339738	-2.03882	-0.2917	H	2.236647	-2.14965	-0.43475
C	2.537699	0.035409	-0.82453	C	2.723252	-0.07016	-0.705
H	3.260035	0.384212	-0.08841	H	3.43421	0.096636	0.102304
H	2.901749	0.01517	-1.84958	H	3.14459	-0.01443	-1.70647
H	1.637377	1.019684	-0.8177	H	1.936767	1.004956	-0.6244
H	0.932154	-1.36746	-1.13419	H	0.9801	-1.20935	-1.25946
O	0.396637	1.267045	0.765744	O	0.577976	1.23275	0.869728
O	0.604168	1.536429	-0.57963	O	0.931245	1.586813	-0.42509
E_{0K}=-496.6218015				E_{0K}=-496.6191118			

Structure 3				Structure 4			
C	-2.6755	0.505763	1.524466	C	-2.50158	-2.22209	-0.74701
H	-2.85372	-0.44881	2.024232	H	-3.29962	-1.48242	-0.67614
H	-2.04989	1.132376	2.162931	H	-2.1049	-2.20532	-1.76312

H	-3.634	1.013627	1.402423	H	-2.91884	-3.21133	-0.55106
C	-2.0441	0.28894	0.159061	C	-1.40558	-1.91074	0.248021
H	-2.73044	-0.24123	-0.50066	H	-1.79215	-1.9151	1.275284
H	-1.78017	1.241023	-0.30761	H	-0.59652	-2.64664	0.191639
O	-0.88675	-0.54888	0.199551	O	-0.90073	-0.61515	-0.05913
C	0.132391	-0.13432	1.024165	C	0.025786	-0.1562	0.849961
H	-0.12384	-0.15328	2.08679	H	-0.34953	-0.16519	1.878106
O	1.211748	-0.97534	0.873588	O	1.185847	-0.92832	0.881454
C	1.725327	-1.15709	-0.44783	C	1.885235	-1.10681	-0.3509
H	2.348477	-2.05303	-0.38603	H	2.545718	-1.9617	-0.18185
C	2.536411	0.0308	-0.88638	C	2.671352	0.120616	-0.71968
H	3.299343	0.357925	-0.18193	H	3.294598	0.529516	0.073423
H	2.845768	0.031993	-1.92947	H	3.128417	0.111339	-1.70674
H	1.644305	1.017177	-0.81196	H	1.692031	1.034769	-0.82442
H	0.905454	-1.35377	-1.14203	H	1.181419	-1.365	-1.14855
O	0.464948	1.241433	0.826087	O	0.273816	1.205649	0.602997
O	0.618915	1.528305	-0.52342	O	0.592955	1.424878	-0.72995
E_{0K}=-496.6196443				E_{0K}=-496.6183148			

Structure 5				Structure 6			
C	-2.1333	-1.91118	1.675617	C	-0.62202	-3.0985	0.004212
H	-1.3839	-1.88701	2.468893	H	-0.49286	-3.08836	-1.07986
H	-2.8627	-1.11798	1.850939	H	0.358105	-3.13671	0.480627
H	-2.64719	-2.87222	1.738148	H	-1.17243	-4.00299	0.272918
C	-1.50658	-1.76174	0.298429	C	-1.40443	-1.87357	0.448563
H	-0.7059	-2.49614	0.16175	H	-2.40196	-1.88066	0.007853
H	-2.25215	-1.91879	-0.4805	H	-1.51768	-1.85938	1.539126
O	-1.00721	-0.45082	0.04217	O	-0.81457	-0.64929	0.014688
C	-0.01542	-0.02397	0.898112	C	0.084952	-0.09612	0.896824
H	-0.34003	0.050201	1.938754	H	-0.29365	-0.0709	1.923074
O	1.087047	-0.87659	0.922006	O	1.288182	-0.79637	0.973886
C	1.739011	-1.14093	-0.32152	C	2.023241	-0.97477	-0.23797
H	2.342306	-2.03502	-0.14123	H	2.728512	-1.78378	-0.02667
C	2.597428	0.01639	-0.75006	C	2.743528	0.282752	-0.63719
H	3.261582	0.412955	0.01556	H	3.313469	0.766529	0.153817
H	3.033027	-0.06108	-1.74381	H	3.231412	0.258819	-1.60915
H	1.675695	0.987214	-0.87513	H	1.709162	1.122809	-0.81313
H	0.999105	-1.37182	-1.09445	H	1.352682	-1.3028	-1.03779
O	0.312648	1.305507	0.576922	O	0.260593	1.264338	0.582516
O	0.604618	1.444884	-0.77264	O	0.582281	1.432163	-0.75696
E_{0K}=-496.6158752				E_{0K}=-496.6158873			

Structure 7

C	-2.31855	-0.79613	-2.00603
H	-2.92364	-1.49803	-1.43063
H	-2.78508	0.188247	-1.95452
H	-2.29819	-1.12127	-3.0479
C	-0.91172	-0.73771	-1.45061
H	-0.44213	-1.72573	-1.48787
H	-0.30294	-0.02295	-2.01088
O	-1.02368	-0.32263	-0.09115
C	0.09637	-0.19563	0.697361
H	-0.22107	-0.35019	1.728617
O	1.096646	-1.13744	0.465294
C	2.096259	-1.00477	-0.54656
H	2.70715	-1.90383	-0.42226
C	2.949425	0.224647	-0.42085
H	3.305347	0.457335	0.581199
H	3.682178	0.35284	-1.2145
H	2.042122	1.19263	-0.60469
H	1.652757	-1.0452	-1.54518
O	0.573486	1.139442	0.735941
O	0.933469	1.566499	-0.53452
E_{0K}=-496.6096632			

(10) T1 diagnostic values for reactants, products and transition states

Table S55. T1 diagnostic values for the lowest energy structures of reactants, products and transition states.

Species	Reactant 1	Product 1	Product 2	Transition state 1	Transition state 2
T1	0.01490897	0.01122069	0.01066586	0.0171889	0.01572767
Species	Reactant 2	Product 3	Product 4	Transition state 3	Transition state 4
T1	0.01447493	0.01073409	0.00837410	0.01806940	0.01557074