

Supplementary Material for

Multi-structural variational kinetics study on hydrogen abstraction reactions of cyclopentanol and cyclopentane by hydroperoxyl radical with anharmonicity, recrossing and tunneling effects

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CONTENTS

1. T1 diagnostic values for reaction species and saddle points.....	- 2 -
2. Electronic structure benchmark calculations by different model chemistries	- 3 -
3. Conformational-rotational-vibrational partition functions	- 11 -
4. Multistructural torsional anharmonicity factors.....	- 19 -
5. Thermodynamic properties for reactant and each transition state using three models	- 24 -
6. Location of generalized transition state at different temperatures.....	- 29 -
7. Transmission coefficients.....	- 31 -
8. Changes of vibrational frequencies along the reaction coordinate	- 36 -
9. Vibrationally adiabatic ground energy along MEPs	- 37 -
10. Tabulated rate constants using different methods	- 38 -
11. Fitting parameters of modified Arrhenius equations.....	- 48 -
12. Temperature-dependent activation energies.....	- 49 -
13. Optimized geometries and calculated non-scaled frequencies	- 52 -

1. T1 diagnostic values for reaction species and saddle points

Table S1 T1 diagnostic values for reaction species and saddle points calculated at the level of CCSD(T)-F12/jun-cc-pVTZ.

	R1	R2a	R2b	R3a	R3b	R4	R_{cpt}
saddle points	0.019	0.018	0.017	0.018	0.016	0.033	0.016
products	0.013	0.012	0.012	0.011	0.011	0.017	0.011
cyclopentanol	0.010						-
cyclopentane	-	-	-	-	-	-	0.009
hydroperoxyl radical	0.029						
hydroperoxide	0.011						

2. Electronic structure benchmark calculations by different model chemistries

Table S2 Forward (V_f^\ddagger) and reverse (V_r^\ddagger) barrier heights, reaction energies (ΔV) and minimum mean unsigned deviations (MUDs) from the coupled cluster benchmark for cyclopentanol + HO₂ and cyclopentane +HO₂ (units: kcal/mol).

Reaction	Method	Basis Set	V_f^\ddagger	V_r^\ddagger	ΔV	MUDs
R1	CCSD(T)-F12	jun-cc-pVTZ	12.22	5.83	6.39	0.00
		MG3S	11.42	5.24	6.18	0.53
		ma-TZVP	12.78	5.81	6.96	0.38
		maug-cc-pVTZ	12.03	6.01	6.01	0.25
		jun-cc-pVTZ	11.96	5.94	6.02	0.25
		jul-cc-pVTZ	11.89	5.90	5.98	0.27
		aug-cc-pVTZ	11.81	5.84	5.97	0.28
	M08-HX	MG3S	11.64	5.88	5.76	0.42
		ma-TZVP	12.99	6.03	6.96	0.52
		maug-cc-pVTZ	12.64	6.50	6.14	0.45
		jun-cc-pVTZ	12.61	6.46	6.16	0.42
		jul-cc-pVTZ	12.46	6.35	6.11	0.35
		aug-cc-pVTZ	12.41	6.30	6.12	0.31
	M08-SO	MG3S	10.17	3.88	6.29	1.37
		ma-TZVP	10.87	4.08	6.79	1.16
		maug-cc-pVTZ	10.35	4.47	5.89	1.24
		jun-cc-pVTZ	10.34	4.43	5.91	1.25
		jul-cc-pVTZ	10.28	4.42	5.86	1.29
		aug-cc-pVTZ	10.22	4.40	5.82	1.33
	M06-2X	MG3S	10.79	3.56	7.23	1.51
		ma-TZVP	11.42	3.50	7.92	1.55

R2a		maug-cc-pVTZ	10.90	4.08	6.81	1.16
		jul-cc-pVTZ	10.86	4.03	6.82	1.20
		aug-cc-pVTZ	10.79	4.04	6.75	1.19
		MG3S	10.66	6.05	4.60	1.19
		ma-TZVP	11.37	5.98	5.39	0.66
	MN15	maug-cc-pVTZ	11.34	6.72	4.62	1.18
		jul-cc-pVTZ	11.30	6.68	4.62	1.18
		jul-cc-pVTZ	11.10	6.50	4.60	1.19
		aug-cc-pVTZ	11.03	6.41	4.63	1.17
	CCSD(T)-F12	jul-cc-pVTZ	16.35	6.19	10.16	0.00
	M08-HX	MG3S	15.22	4.50	10.72	1.13
		ma-TZVP	17.07	5.29	11.77	1.08
		maug-cc-pVTZ	16.04	5.59	10.44	0.39
		jul-cc-pVTZ	15.84	5.34	10.50	0.56
		jul-cc-pVTZ	15.84	5.35	10.49	0.56
		aug-cc-pVTZ	15.77	5.30	10.47	0.59
	M08-SO	MG3S	15.26	6.07	9.19	0.73
		ma-TZVP	17.31	6.57	10.73	0.64
		maug-cc-pVTZ	16.77	7.15	9.63	0.64
		jul-cc-pVTZ	16.62	6.90	9.73	0.47
		jul-cc-pVTZ	16.51	6.82	9.70	0.42
		aug-cc-pVTZ	16.44	6.77	9.67	0.39
	M06-2X	MG3S	13.86	3.49	10.38	1.80
		ma-TZVP	14.85	3.88	10.98	1.54
		maug-cc-pVTZ	14.20	4.35	9.85	1.43
		jul-cc-pVTZ	14.09	4.16	9.93	1.50
		jul-cc-pVTZ	14.07	4.19	9.88	1.52
		aug-cc-pVTZ	14.01	4.18	9.83	1.55

R2b	M05-2X	MG3S	14.64	3.59	11.05	1.73
		ma-TZVP	15.58	3.66	11.92	1.68
		maug-cc-pVTZ	14.85	4.33	10.52	1.24
		jun-cc-pVTZ	14.72	4.15	10.58	1.36
		jul-cc-pVTZ	14.70	4.20	10.51	1.32
		aug-cc-pVTZ	14.63	4.18	10.44	1.33
	MN15	MG3S	13.95	4.98	8.98	1.59
		ma-TZVP	15.18	5.22	9.96	0.78
		maug-cc-pVTZ	14.87	5.89	8.98	0.99
		jun-cc-pVTZ	14.75	5.71	9.04	1.06
		jul-cc-pVTZ	14.59	5.53	9.06	1.17
		aug-cc-pVTZ	14.48	5.49	8.99	1.25
	CCSD(T)-F12	jun-cc-pVTZ	18.73	7.46	11.27	0.00
	M08-HX	MG3S	18.65	6.86	11.78	0.40
		ma-TZVP	20.07	7.27	12.80	1.02
		maug-cc-pVTZ	19.14	7.64	11.50	0.27
		jun-cc-pVTZ	19.10	7.56	11.54	0.25
		jul-cc-pVTZ	19.06	7.54	11.52	0.22
		aug-cc-pVTZ	18.95	7.43	11.51	0.16
	M08-SO	MG3S	18.98	8.29	10.69	0.56
		ma-TZVP	20.41	8.28	12.12	1.12
		maug-cc-pVTZ	19.99	8.88	11.11	0.95
		jun-cc-pVTZ	20.00	8.82	11.18	0.91
		jul-cc-pVTZ	19.88	8.75	11.13	0.86
		aug-cc-pVTZ	19.80	8.67	11.13	0.81
	M06-2X	MG3S	17.18	5.63	11.55	1.22
		ma-TZVP	17.96	5.78	12.18	1.12
		maug-cc-pVTZ	17.27	6.23	11.04	0.97
		jun-cc-pVTZ	17.29	6.18	11.11	0.96

		jul-cc-pVTZ	17.24	6.19	11.04	1.00
		aug-cc-pVTZ	17.16	6.16	11.01	1.04
		MG3S	17.54	5.22	12.32	1.49
		ma-TZVP	18.17	4.99	13.19	1.65
	M05-2X	maug-cc-pVTZ	17.44	5.66	11.78	1.20
		jul-cc-pVTZ	17.45	5.63	11.83	1.22
		jul-cc-pVTZ	17.39	5.65	11.74	1.20
		aug-cc-pVTZ	17.29	5.60	11.69	1.24
		MG3S	17.70	7.42	10.29	0.69
		ma-TZVP	18.44	7.21	11.23	0.20
	MN15	maug-cc-pVTZ	18.18	7.92	10.25	0.68
		jul-cc-pVTZ	18.19	7.89	10.30	0.65
		jul-cc-pVTZ	18.02	7.74	10.28	0.66
		aug-cc-pVTZ	17.93	7.67	10.26	0.68
	CCSD(T)-F12	jul-cc-pVTZ	13.53	3.76	9.77	0.00
		MG3S	12.58	2.62	9.96	0.76
		ma-TZVP	14.22	3.21	11.02	0.83
	M08-HX	maug-cc-pVTZ	13.33	3.61	9.71	0.14
		jul-cc-pVTZ	13.26	3.50	9.76	0.18
		jul-cc-pVTZ	13.24	3.50	9.74	0.19
		aug-cc-pVTZ	13.14	3.43	9.71	0.26
R3a		MG3S	12.53	3.63	8.90	0.67
		ma-TZVP	14.31	3.92	10.39	0.52
	M08-SO	maug-cc-pVTZ	13.98	4.55	9.43	0.53
		jul-cc-pVTZ	13.95	4.43	9.52	0.45
		jul-cc-pVTZ	13.83	4.37	9.47	0.41
		aug-cc-pVTZ	13.74	4.31	9.43	0.37
	M06-2X	MG3S	11.18	1.21	9.97	1.70
		ma-TZVP	12.01	1.37	10.64	1.59

R3b		maug-cc-pVTZ	11.46	1.97	9.49	1.38
		jun-cc-pVTZ	11.45	1.89	9.56	1.39
		jul-cc-pVTZ	11.40	1.90	9.50	1.42
		aug-cc-pVTZ	11.33	1.89	9.45	1.46
	M05-2X	MG3S	11.84	1.27	10.57	1.66
		ma-TZVP	12.61	1.10	11.51	1.77
		maug-cc-pVTZ	11.99	1.89	10.11	1.25
		jun-cc-pVTZ	11.96	1.81	10.15	1.30
		jul-cc-pVTZ	11.91	1.84	10.07	1.28
		aug-cc-pVTZ	11.81	1.81	10.00	1.30
	MN15	MG3S	11.52	3.19	8.33	1.34
		ma-TZVP	12.54	3.20	9.34	0.66
		maug-cc-pVTZ	12.38	3.99	8.39	0.92
		jun-cc-pVTZ	12.36	3.92	8.44	0.89
		jul-cc-pVTZ	12.17	3.76	8.42	0.91
		aug-cc-pVTZ	12.03	3.68	8.35	1.00
	CCSD(T)-F12	jun-cc-pVTZ	18.20	7.76	10.43	0.00
	M08-HX	MG3S	17.68	6.96	10.72	0.53
		ma-TZVP	19.07	7.40	11.67	0.82
		maug-cc-pVTZ	18.18	7.76	10.42	0.01
		jun-cc-pVTZ	18.16	7.70	10.46	0.05
		jul-cc-pVTZ	18.11	7.68	10.44	0.06
		aug-cc-pVTZ	18.00	7.58	10.42	0.13
	M08-SO	MG3S	18.15	8.29	9.86	0.38
		ma-TZVP	19.54	8.32	11.22	0.89
		maug-cc-pVTZ	19.19	8.91	10.29	0.76
		jun-cc-pVTZ	19.22	8.86	10.36	0.73
		jul-cc-pVTZ	19.10	8.79	10.31	0.69

R4	M06-2X	aug-cc-pVTZ	19.03	8.73	10.30	0.64
		MG3S	16.35	5.68	10.67	1.39
		ma-TZVP	17.11	5.81	11.30	1.31
		maug-cc-pVTZ	16.46	6.28	10.18	1.16
		jun-cc-pVTZ	16.49	6.24	10.25	1.14
		jul-cc-pVTZ	16.43	6.25	10.18	1.18
		aug-cc-pVTZ	16.35	6.22	10.14	1.23
	M05-2X	MG3S	16.73	5.39	11.34	1.58
		ma-TZVP	17.34	5.12	12.21	1.76
		maug-cc-pVTZ	16.65	5.81	10.83	1.30
		jun-cc-pVTZ	16.66	5.80	10.87	1.31
		jul-cc-pVTZ	16.60	5.82	10.78	1.30
		aug-cc-pVTZ	16.50	5.77	10.72	1.33
	MN15	MG3S	16.90	7.69	9.21	0.86
		ma-TZVP	17.62	7.47	10.15	0.39
		maug-cc-pVTZ	17.40	8.19	9.21	0.81
		jun-cc-pVTZ	17.43	8.18	9.25	0.79
		jul-cc-pVTZ	17.26	8.02	9.24	0.80
		aug-cc-pVTZ	17.17	7.96	9.20	0.82
	M08-HX	CCSD(T)-F12 jun-cc-pVTZ	22.20	4.98	17.22	0.00
		MG3S	21.37	3.64	17.73	0.89
		ma-TZVP	22.54	4.25	18.29	0.71
		maug-cc-pVTZ	21.82	4.16	17.66	0.54
		jun-cc-pVTZ	21.80	4.14	17.66	0.56
		jul-cc-pVTZ	21.75	4.12	17.63	0.58
		aug-cc-pVTZ	21.67	4.06	17.60	0.61
	M08-SO	MG3S	20.32	3.07	17.25	1.27
		ma-TZVP	21.15	3.45	17.70	1.02

		maug-cc-pVTZ	21.20	3.71	17.49	0.85
		jun-cc-pVTZ	21.22	3.69	17.53	0.86
		jul-cc-pVTZ	21.14	3.61	17.54	0.92
		aug-cc-pVTZ	21.09	3.57	17.52	0.94
	M06-2X	MG3S	18.78	1.66	17.12	2.28
		ma-TZVP	19.51	2.05	17.47	1.95
		maug-cc-pVTZ	19.03	2.06	16.98	2.11
		jun-cc-pVTZ	19.05	2.06	16.99	2.10
		jul-cc-pVTZ	19.01	2.07	16.95	2.12
		aug-cc-pVTZ	18.96	2.04	16.92	2.16
		M05-2X	MG3S	20.38	2.68	17.71
	ma-TZVP		20.84	2.65	18.19	1.55
	maug-cc-pVTZ		20.43	2.89	17.55	1.39
	jun-cc-pVTZ		20.44	2.89	17.54	1.39
	jul-cc-pVTZ		20.39	2.90	17.49	1.39
	aug-cc-pVTZ		20.31	2.85	17.45	1.42
	MN15		MG3S	18.20	1.78	16.42
		ma-TZVP	18.66	1.89	16.76	2.36
		maug-cc-pVTZ	18.67	2.18	16.49	2.35
		jun-cc-pVTZ	18.67	2.19	16.48	2.35
		jul-cc-pVTZ	18.59	2.12	16.48	2.40
		aug-cc-pVTZ	18.52	2.06	16.46	2.45
		CCSD(T)-F12	jun-cc-pVTZ	18.07	7.81	10.26
		MG3S	17.72	7.15	10.57	0.44
		ma-TZVP	19.14	7.61	11.53	0.85
<i>Rcpt</i>	M08-HX	maug-cc-pVTZ	18.18	7.91	10.28	0.08
		jun-cc-pVTZ	18.15	7.84	10.32	0.06
		jul-cc-pVTZ	18.10	7.81	10.29	0.02

	aug-cc-pVTZ	17.99	7.72	10.27	0.06
M08-SO	MG3S	17.88	8.00	9.89	0.25
	ma-TZVP	19.33	8.03	11.30	0.84
	maug-cc-pVTZ	18.85	8.51	10.34	0.52
	jun-cc-pVTZ	18.86	8.45	10.41	0.52
	jul-cc-pVTZ	18.74	8.38	10.36	0.44
	aug-cc-pVTZ	18.66	8.33	10.33	0.39
M06-2X	MG3S	16.32	5.80	10.52	1.34
	ma-TZVP	17.08	5.94	11.14	1.24
	maug-cc-pVTZ	16.39	6.36	10.03	1.12
	jun-cc-pVTZ	16.40	6.31	10.09	1.11
	jul-cc-pVTZ	16.34	6.32	10.02	1.15
	aug-cc-pVTZ	16.27	6.29	9.98	1.20
M05-2X	MG3S	16.69	5.52	11.17	1.53
	ma-TZVP	17.31	5.27	12.04	1.69
	maug-cc-pVTZ	16.58	5.92	10.66	1.26
	jun-cc-pVTZ	16.58	5.89	10.70	1.28
	jul-cc-pVTZ	16.52	5.91	10.61	1.27
	aug-cc-pVTZ	16.42	5.87	10.56	1.29
MN15	MG3S	16.85	7.79	9.05	0.82
	ma-TZVP	17.59	7.59	9.99	0.32
	maug-cc-pVTZ	17.32	8.27	9.05	0.81
	jun-cc-pVTZ	17.34	8.25	9.09	0.78
	jul-cc-pVTZ	17.18	8.10	9.08	0.79
	aug-cc-pVTZ	17.08	8.04	9.04	0.81

3. Conformational-rotational-vibrational partition functions

Table S3 Conformational-rotational-vibrational partition functions with the multi-structural torsional (MS-T) approximation, the multi-structural local harmonic (MS-LH) approximation, and the single-structure quasi-harmonic (SS-QH) approximation.

T (K)	$Q_{\text{con-rovib}}^{\text{MS-T}}$	$Q_{\text{con-rovib}}^{\text{MS-LH}}$	$Q_{\text{rovib,l}}^{\text{SS-QH}}$
CPL			
200	1.51E-91	1.95E-91	3.87E-92
250	1.07E-71	1.41E-71	2.69E-72
300	2.41E-58	3.23E-58	6.00E-59
350	1.06E-48	1.45E-48	2.64E-49
400	2.25E-41	3.15E-41	5.66E-42
450	1.38E-35	1.97E-35	3.50E-36
500	7.08E-31	1.03E-30	1.81E-31
550	5.97E-27	8.87E-27	1.55E-27
600	1.30E-23	1.97E-23	3.42E-24
650	9.96E-21	1.54E-20	2.66E-21
700	3.36E-18	5.28E-18	9.08E-19
750	5.84E-16	9.36E-16	1.60E-16
800	5.93E-14	9.68E-14	1.65E-14
850	3.86E-12	6.41E-12	1.09E-12
900	1.73E-10	2.92E-10	4.95E-11
950	5.63E-09	9.66E-09	1.64E-09
1000	1.40E-07	2.44E-07	4.13E-08
1100	4.41E-05	7.94E-05	1.34E-05
1200	6.77E-03	1.25E-02	2.11E-03
1300	5.91E-01	1.13E+00	1.89E-01
1400	3.28E+01	6.42E+01	1.07E+01
1500	1.26E+03	2.52E+03	4.21E+02

1600	3.54E+04	7.28E+04	1.21E+04
1700	7.70E+05	1.62E+06	2.70E+05
1800	1.34E+07	2.88E+07	4.80E+06
1900	1.93E+08	4.24E+08	7.04E+07
2000	2.35E+09	5.26E+09	8.73E+08
SP1			
200	2.58E-98	4.74E-98	1.10E-98
250	1.46E-76	2.67E-76	5.10E-77
300	7.54E-62	1.37E-61	2.19E-62
350	3.67E-51	6.59E-51	9.02E-52
400	5.39E-43	9.53E-43	1.14E-43
450	1.64E-36	2.86E-36	3.03E-37
500	3.29E-31	5.64E-31	5.39E-32
550	9.07E-27	1.53E-26	1.34E-27
600	5.61E-23	9.35E-23	7.54E-24
650	1.09E-19	1.80E-19	1.35E-20
700	8.52E-17	1.39E-16	9.81E-18
750	3.18E-14	5.14E-14	3.44E-15
800	6.51E-12	1.04E-11	6.64E-13
850	8.08E-10	1.29E-09	7.83E-11
900	6.57E-08	1.04E-07	6.09E-09
950	3.74E-06	5.93E-06	3.33E-07
1000	1.57E-04	2.48E-04	1.35E-05
1100	1.28E-01	2.02E-01	1.03E-02
1200	4.57E+01	7.28E+01	3.54E+00
1300	8.57E+03	1.38E+04	6.41E+02
1400	9.54E+05	1.55E+06	6.94E+04
1500	6.92E+07	1.14E+08	4.94E+06
1600	3.51E+09	5.86E+09	2.47E+08

1700	1.32E+11	2.24E+11	9.17E+09
1800	3.81E+12	6.59E+12	2.64E+11
1900	8.82E+13	1.56E+14	6.10E+12
2000	1.68E+15	3.02E+15	1.16E+14
SP2a			
200	2.86E-99	4.94E-99	1.89E-99
250	1.58E-77	2.75E-77	7.68E-78
300	8.76E-63	1.53E-62	2.98E-63
350	4.71E-52	8.18E-52	1.13E-52
400	7.67E-44	1.32E-43	1.33E-44
450	2.57E-37	4.39E-37	3.37E-38
500	5.64E-32	9.50E-32	5.76E-33
550	1.68E-27	2.80E-27	1.38E-28
600	1.11E-23	1.83E-23	7.58E-25
650	2.30E-20	3.75E-20	1.33E-21
700	1.89E-17	3.06E-17	9.47E-19
750	7.43E-15	1.19E-14	3.27E-16
800	1.59E-12	2.54E-12	6.23E-14
850	2.05E-10	3.26E-10	7.26E-12
900	1.73E-08	2.75E-08	5.60E-10
950	1.02E-06	1.61E-06	3.04E-08
1000	4.38E-05	6.95E-05	1.22E-06
1100	3.77E-02	6.00E-02	9.25E-04
1200	1.41E+01	2.27E+01	3.14E-01
1300	2.76E+03	4.46E+03	5.63E+01
1400	3.18E+05	5.21E+05	6.06E+03
1500	2.38E+07	3.95E+07	4.29E+05
1600	1.24E+09	2.10E+09	2.14E+07
1700	4.78E+10	8.20E+10	7.91E+08

1800	1.42E+12	2.47E+12	2.27E+10
1900	3.35E+13	5.96E+13	5.24E+11
2000	6.49E+14	1.18E+15	9.95E+12
SP2b			
200	8.47E-97	1.32E-96	9.93E-98
250	3.32E-75	5.00E-75	3.33E-76
300	1.29E-60	1.90E-60	1.16E-61
350	4.95E-50	7.23E-50	4.11E-51
400	5.95E-42	8.64E-42	4.65E-43
450	1.53E-35	2.22E-35	1.14E-36
500	2.65E-30	3.85E-30	1.92E-31
550	6.43E-26	9.38E-26	4.53E-27
600	3.55E-22	5.22E-22	2.46E-23
650	6.26E-19	9.27E-19	4.28E-20
700	4.47E-16	6.69E-16	3.03E-17
750	1.54E-13	2.34E-13	1.04E-14
800	2.94E-11	4.50E-11	1.98E-12
850	3.41E-09	5.30E-09	2.30E-10
900	2.62E-07	4.12E-07	1.77E-08
950	1.41E-05	2.26E-05	9.57E-07
1000	5.61E-04	9.12E-04	3.83E-05
1100	4.18E-01	7.03E-01	2.91E-02
1200	1.39E+02	2.41E+02	9.84E+00
1300	2.43E+04	4.38E+04	1.77E+03
1400	2.55E+06	4.76E+06	1.90E+05
1500	1.75E+08	3.40E+08	1.34E+07
1600	8.50E+09	1.71E+10	6.70E+08
1700	3.06E+11	6.36E+11	2.48E+10
1800	8.52E+12	1.84E+13	7.12E+11

1900	1.91E+14	4.26E+14	1.64E+13
2000	3.51E+15	8.14E+15	3.12E+14
SP3a			
200	2.93E-99	4.74E-99	2.08E-99
250	1.37E-77	2.15E-77	8.32E-78
300	6.48E-63	9.82E-63	3.19E-63
350	3.10E-52	4.57E-52	1.20E-52
400	4.74E-44	6.89E-44	1.40E-44
450	1.55E-37	2.26E-37	3.52E-38
500	3.40E-32	5.04E-32	5.99E-33
550	1.03E-27	1.57E-27	1.43E-28
600	7.00E-24	1.10E-23	7.80E-25
650	1.49E-20	2.43E-20	1.36E-21
700	1.27E-17	2.14E-17	9.66E-19
750	5.11E-15	8.95E-15	3.32E-16
800	1.12E-12	2.04E-12	6.31E-14
850	1.48E-10	2.79E-10	7.34E-12
900	1.28E-08	2.50E-08	5.64E-10
950	7.69E-07	1.55E-06	3.05E-08
1000	3.38E-05	7.06E-05	1.22E-06
1100	3.00E-02	6.68E-02	9.25E-04
1200	1.16E+01	2.74E+01	3.13E-01
1300	2.30E+03	5.78E+03	5.60E+01
1400	2.70E+05	7.17E+05	6.02E+03
1500	2.05E+07	5.74E+07	4.25E+05
1600	1.08E+09	3.19E+09	2.11E+07
1700	4.21E+10	1.30E+11	7.82E+08
1800	1.26E+12	4.08E+12	2.24E+10
1900	2.99E+13	1.02E+14	5.16E+11

2000	5.83E+14	2.07E+15	9.81E+12
SP3b			
200	6.24E-97	9.31E-97	5.32E-98
250	2.45E-75	3.53E-75	1.80E-76
300	9.63E-61	1.34E-60	6.29E-62
350	3.76E-50	5.11E-50	2.24E-51
400	4.60E-42	6.11E-42	2.55E-43
450	1.20E-35	1.57E-35	6.27E-37
500	2.12E-30	2.72E-30	1.05E-31
550	5.23E-26	6.64E-26	2.49E-27
600	2.93E-22	3.69E-22	1.35E-23
650	5.23E-19	6.56E-19	2.36E-20
700	3.78E-16	4.73E-16	1.67E-17
750	1.32E-13	1.65E-13	5.73E-15
800	2.54E-11	3.18E-11	1.09E-12
850	2.98E-09	3.74E-09	1.27E-10
900	2.31E-07	2.91E-07	9.74E-09
950	1.26E-05	1.59E-05	5.27E-07
1000	5.04E-04	6.43E-04	2.11E-05
1100	3.81E-01	4.95E-01	1.60E-02
1200	1.28E+02	1.70E+02	5.41E+00
1300	2.27E+04	3.08E+04	9.71E+02
1400	2.41E+06	3.35E+06	1.05E+05
1500	1.67E+08	2.39E+08	7.39E+06
1600	8.16E+09	1.20E+10	3.68E+08
1700	2.96E+11	4.47E+11	1.36E+10
1800	8.29E+12	1.29E+13	3.91E+11
1900	1.87E+14	2.99E+14	9.01E+12
2000	3.46E+15	5.72E+15	1.71E+14

SP4			
200	9.23E-97	1.42E-96	3.81E-97
250	3.52E-75	5.27E-75	1.21E-75
300	1.36E-60	1.98E-60	3.98E-61
350	5.20E-50	7.39E-50	1.34E-50
400	6.27E-42	8.70E-42	1.45E-42
450	1.62E-35	2.19E-35	3.42E-36
500	2.82E-30	3.74E-30	5.52E-31
550	6.88E-26	8.97E-26	1.26E-26
600	3.83E-22	4.91E-22	6.62E-23
650	6.80E-19	8.59E-19	1.12E-19
700	4.90E-16	6.11E-16	7.71E-17
750	1.70E-13	2.10E-13	2.58E-14
800	3.27E-11	4.00E-11	4.80E-12
850	3.84E-09	4.66E-09	5.47E-10
900	2.97E-07	3.58E-07	4.13E-08
950	1.61E-05	1.94E-05	2.20E-06
1000	6.48E-04	7.77E-04	8.67E-05
1100	4.91E-01	5.89E-01	6.40E-02
1200	1.66E+02	1.99E+02	2.12E+01
1300	2.95E+04	3.58E+04	3.73E+03
1400	3.15E+06	3.85E+06	3.95E+05
1500	2.20E+08	2.73E+08	2.75E+07
1600	1.08E+10	1.36E+10	1.35E+09
1700	3.93E+11	5.03E+11	4.96E+10
1800	1.11E+13	1.45E+13	1.41E+12
1900	2.51E+14	3.34E+14	3.23E+13
2000	4.69E+15	6.36E+15	6.10E+14

SPc_{pt}

200	1.66E-94	2.67E-94	6.13E-95
250	1.14E-73	1.82E-73	3.94E-74
300	1.31E-59	2.05E-59	4.25E-60
350	2.01E-49	3.08E-49	6.20E-50
400	1.17E-41	1.76E-41	3.46E-42
450	1.66E-35	2.46E-35	4.74E-36
500	1.75E-30	2.55E-30	4.83E-31
550	2.76E-26	3.98E-26	7.44E-27
600	1.05E-22	1.49E-22	2.77E-23
650	1.33E-19	1.87E-19	3.43E-20
700	7.08E-17	9.87E-17	1.79E-17
750	1.87E-14	2.59E-14	4.68E-15
800	2.80E-12	3.85E-12	6.90E-13
850	2.60E-10	3.56E-10	6.35E-11
900	1.63E-08	2.22E-08	3.93E-09
950	7.25E-07	9.85E-07	1.74E-07
1000	2.42E-05	3.28E-05	5.77E-06
1100	1.31E-02	1.77E-02	3.10E-03
1200	3.27E+00	4.44E+00	7.72E-01
1300	4.44E+02	6.06E+02	1.05E+02
1400	3.70E+04	5.08E+04	8.76E+03
1500	2.06E+06	2.86E+06	4.90E+05
1600	8.22E+07	1.15E+08	1.97E+07
1700	2.47E+09	3.50E+09	5.96E+08
1800	5.82E+10	8.34E+10	1.42E+10
1900	1.11E+12	1.62E+12	2.74E+11
2000	1.77E+13	2.61E+13	4.42E+12

4. Multistructural torsional anharmonicity factors

Table S4 Multistructural torsional anharmonicity (MS-T) factors for cyclopentanol and saddle points in cyclopentanol + HO₂ and cyclopentane +HO₂.

<i>T</i> (K)	cyclopentanol	SP1	SP2a	SP2b	SP3a	SP3b	SP4	SP _{cpt}
200	3.91	2.35	1.51	8.53	1.41	11.72	2.42	2.70
250	3.99	2.86	2.06	9.96	1.65	13.62	2.92	2.91
300	4.01	3.43	2.94	11.12	2.03	15.30	3.41	3.08
350	4.01	4.07	4.18	12.05	2.60	16.78	3.87	3.24
400	3.98	4.73	5.76	12.79	3.38	18.07	4.32	3.38
450	3.95	5.42	7.64	13.38	4.40	19.19	4.73	3.51
500	3.90	6.10	9.78	13.83	5.69	20.14	5.11	3.62
550	3.85	6.78	12.14	14.19	7.22	20.96	5.46	3.72
600	3.80	7.44	14.65	14.45	8.98	21.64	5.79	3.80
650	3.75	8.08	17.29	14.63	10.95	22.21	6.09	3.88
700	3.69	8.69	19.99	14.76	13.10	22.68	6.36	3.95
750	3.64	9.27	22.73	14.83	15.38	23.05	6.60	4.01
800	3.59	9.81	25.47	14.85	17.76	23.34	6.82	4.06
850	3.54	10.32	28.19	14.84	20.21	23.56	7.01	4.10
900	3.49	10.79	30.86	14.79	22.69	23.72	7.19	4.13
950	3.44	11.23	33.46	14.72	25.18	23.81	7.34	4.16
1000	3.39	11.63	35.98	14.63	27.65	23.86	7.47	4.19
1100	3.30	12.33	40.75	14.38	32.46	23.83	7.68	4.22
1200	3.21	12.91	45.10	14.09	36.98	23.65	7.83	4.23
1300	3.13	13.38	49.00	13.76	41.14	23.38	7.92	4.23
1400	3.06	13.74	52.47	13.41	44.91	23.03	7.97	4.22
1500	2.98	14.01	55.50	13.05	48.27	22.62	7.98	4.20
1600	2.92	14.21	58.14	12.69	51.22	22.17	7.96	4.17
1700	2.86	14.35	60.40	12.32	53.78	21.70	7.92	4.14
1800	2.80	14.42	62.32	11.97	55.99	21.20	7.86	4.10

1900	2.74	14.45	63.93	11.61	57.86	20.70	7.78	4.05
2000	2.69	14.44	65.26	11.27	59.42	20.20	7.68	4.01

Table S5 Multistructural local harmonic (MS-LH) factors for cyclopentanol and saddle points in cyclopentanol + HO₂ and cyclopentane +HO₂.

<i>T</i> (K)	cyclopentanol	SP1	SP2a	SP2b	SP3a	SP3b	SP4	SP _{cpt}
200	5.037	4.318	2.611	13.246	2.278	17.483	3.714	4.348
250	5.24	5.238	3.574	15.024	2.586	19.626	4.363	4.615
300	5.382	6.248	5.125	16.445	3.079	21.369	4.965	4.815
350	5.486	7.306	7.26	17.606	3.825	22.803	5.507	4.97
400	5.565	8.376	9.921	18.572	4.908	23.998	5.988	5.093
450	5.628	9.433	13.025	19.385	6.414	25.008	6.412	5.193
500	5.678	10.462	16.484	20.08	8.416	25.871	6.788	5.276
550	5.72	11.452	20.215	20.68	10.968	26.616	7.121	5.346
600	5.755	12.399	24.143	21.203	14.1	27.266	7.418	5.405
650	5.785	13.299	28.207	21.663	17.817	27.838	7.684	5.456
700	5.811	14.154	32.353	22.07	22.106	28.345	7.923	5.5
750	5.833	14.963	36.54	22.434	26.939	28.797	8.138	5.539
800	5.852	15.728	40.733	22.76	32.276	29.203	8.334	5.574
850	5.87	16.452	44.905	23.054	38.072	29.57	8.512	5.605
900	5.885	17.137	49.035	23.321	44.278	29.902	8.674	5.632
950	5.899	17.784	53.107	23.565	50.845	30.206	8.823	5.657
1000	5.911	18.397	57.108	23.788	57.723	30.483	8.961	5.68
1100	5.932	19.528	64.864	24.181	72.233	30.973	9.205	5.719
1200	5.95	20.544	72.258	24.518	87.471	31.393	9.415	5.752
1300	5.964	21.462	79.271	24.81	103.154	31.756	9.598	5.78
1400	5.977	22.293	85.902	25.065	119.055	32.074	9.759	5.805
1500	5.988	23.049	92.161	25.29	134.993	32.354	9.901	5.826
1600	5.998	23.739	98.062	25.49	150.829	32.603	10.028	5.845

1700	6.006	24.37	103.624	25.669	166.459	32.826	10.142	5.861
1800	6.013	24.95	108.867	25.83	181.807	33.026	10.244	5.876
1900	6.02	25.484	113.812	25.976	196.816	33.208	10.337	5.89
2000	6.026	25.978	118.479	26.109	211.448	33.373	10.422	5.902

Table S6 Multistructural torsional anharmonicity (MS-T) factors for each studied reaction.

<i>T</i> (K)	R1	R2a	R2b	R3a	R3b	R4	<i>Rcpt</i>
200	0.60	0.39	2.18	0.36	2.99	0.62	2.70
250	0.72	0.52	2.50	0.41	3.42	0.73	2.91
300	0.86	0.73	2.77	0.51	3.81	0.85	3.08
350	1.02	1.04	3.01	0.65	4.19	0.97	3.24
400	1.19	1.45	3.21	0.85	4.54	1.08	3.38
450	1.37	1.94	3.39	1.12	4.86	1.20	3.51
500	1.56	2.51	3.55	1.46	5.16	1.31	3.62
550	1.76	3.15	3.68	1.87	5.44	1.42	3.72
600	1.96	3.86	3.80	2.36	5.70	1.52	3.80
650	2.16	4.61	3.91	2.92	5.93	1.62	3.88
700	2.35	5.41	4.00	3.55	6.14	1.72	3.95
750	2.55	6.24	4.07	4.22	6.33	1.81	4.01
800	2.74	7.10	4.14	4.95	6.51	1.90	4.06
850	2.92	7.97	4.20	5.72	6.67	1.98	4.10
900	3.10	8.85	4.24	6.51	6.81	2.06	4.13
950	3.27	9.74	4.28	7.33	6.93	2.14	4.16
1000	3.43	10.62	4.32	8.16	7.04	2.20	4.19
1100	3.74	12.36	4.36	9.85	7.23	2.33	4.22
1200	4.02	14.04	4.39	11.52	7.37	2.44	4.23
1300	4.27	15.66	4.40	13.14	7.47	2.53	4.23
1400	4.50	17.17	4.39	14.70	7.54	2.61	4.22
1500	4.70	18.60	4.37	16.17	7.58	2.67	4.20

1600	4.87	19.92	4.35	17.55	7.60	2.73	4.17
1700	5.02	21.16	4.32	18.84	7.60	2.77	4.14
1800	5.16	22.29	4.28	20.02	7.58	2.81	4.10
1900	5.27	23.32	4.24	21.11	7.55	2.84	4.05
2000	5.37	24.28	4.19	22.11	7.51	2.86	4.01

Table S7 Multistructural local harmonic (MS-LH) factors for each studied reaction.

<i>T</i> (K)	R1	R2a	R2b	R3a	R3b	R4	<i>R_{cpt}</i>
200	0.86	0.52	2.63	0.45	3.47	0.74	4.35
250	1.00	0.68	2.87	0.49	3.75	0.83	4.62
300	1.16	0.95	3.06	0.57	3.97	0.92	4.82
350	1.33	1.32	3.21	0.70	4.16	1.00	4.97
400	1.51	1.78	3.34	0.88	4.31	1.08	5.09
450	1.68	2.31	3.44	1.14	4.44	1.14	5.19
500	1.84	2.90	3.54	1.48	4.56	1.20	5.28
550	2.00	3.53	3.62	1.92	4.65	1.24	5.35
600	2.15	4.20	3.68	2.45	4.74	1.29	5.41
650	2.30	4.88	3.74	3.08	4.81	1.33	5.46
700	2.44	5.57	3.80	3.80	4.88	1.36	5.50
750	2.57	6.26	3.85	4.62	4.94	1.40	5.54
800	2.69	6.96	3.89	5.52	4.99	1.42	5.57
850	2.80	7.65	3.93	6.49	5.04	1.45	5.61
900	2.91	8.33	3.96	7.52	5.08	1.47	5.63
950	3.01	9.00	3.99	8.62	5.12	1.50	5.66
1000	3.11	9.66	4.02	9.77	5.16	1.52	5.68
1100	3.29	10.93	4.08	12.18	5.22	1.55	5.72
1200	3.45	12.14	4.12	14.70	5.28	1.58	5.75
1300	3.60	13.29	4.16	17.30	5.32	1.61	5.78
1400	3.73	14.37	4.19	19.92	5.37	1.63	5.81

1500	3.85	15.39	4.22	22.54	5.40	1.65	5.83
1600	3.96	16.35	4.25	25.15	5.44	1.67	5.85
1700	4.06	17.25	4.27	27.72	5.47	1.69	5.86
1800	4.15	18.11	4.30	30.24	5.49	1.70	5.88
1900	4.23	18.91	4.31	32.69	5.52	1.72	5.89
2000	4.31	19.66	4.33	35.09	5.54	1.73	5.90

5. Thermodynamic properties for reactant and each transition state using three models

Table S8 Standard-state entropy (S_T^\ominus), heat capacity ($C_p^\ominus(T)$) and relative enthalpy ($H_p^\ominus(T)$)^a of cyclopentanol and each transition state calculated using three models of torsional anharmonicity.

T (K)	S_T^\ominus (cal/mol/K)			$C_p^\ominus(T)$ (cal/mol/K)			$H_p^\ominus(T)$ (kcal/mol)		
	MS-T	MS-LH	SS-QH ^b	MS-T	MS-LH	SS-QH ^b	MS-T	MS-LH	SS-QH ^b
CPL									
200	74.3	75.0	72.7	17.6	17.9	17.9	91.5	91.5	91.5
250	78.6	79.4	77.1	21.2	21.6	21.6	92.5	92.5	92.4
300	82.8	83.7	81.4	25.3	25.8	25.8	93.6	93.7	93.6
350	87.1	88.0	85.7	29.6	30.2	30.2	95.0	95.1	95.0
400	91.3	92.3	90.0	33.9	34.5	34.5	96.6	96.7	96.6
450	95.5	96.6	94.3	37.9	38.6	38.6	98.4	98.6	98.5
500	99.7	100.8	98.6	41.6	42.3	42.3	100.4	100.6	100.5
550	103.8	105.0	102.8	44.9	45.7	45.7	102.5	102.8	102.7
600	107.9	109.1	106.9	48.0	48.8	48.8	104.9	105.1	105.1
650	111.8	113.2	110.9	50.8	51.6	51.6	107.3	107.7	107.6
700	115.7	117.1	114.8	53.3	54.2	54.2	109.9	110.3	110.2
750	119.4	120.9	118.7	55.6	56.5	56.5	112.7	113.1	113.0
800	123.1	124.6	122.4	57.8	58.7	58.7	115.5	115.9	115.9
850	126.6	128.2	126.0	59.8	60.7	60.7	118.4	118.9	118.8
900	130.1	131.8	129.5	61.6	62.5	62.5	121.5	122.0	121.9
950	133.5	135.2	132.9	63.3	64.2	64.2	124.6	125.2	125.1
1000	136.8	138.5	136.3	64.8	65.8	65.8	127.8	128.4	128.3
1100	143.1	144.9	142.7	67.6	68.6	68.6	134.4	135.1	135.1
1200	149.1	151.0	148.8	70.0	71.0	71.0	141.3	142.1	142.0
1300	154.8	156.7	154.5	72.1	73.1	73.1	148.4	149.3	149.3
1400	160.2	162.2	160.0	74.0	74.9	74.9	155.7	156.7	156.7
1500	165.3	167.5	165.2	75.6	76.5	76.5	163.2	164.3	164.2
1600	170.3	172.4	170.2	76.9	77.9	77.9	170.8	172.0	172.0
1700	175.0	177.2	175.0	78.2	79.1	79.1	178.6	179.9	179.8
1800	179.5	181.8	179.5	79.2	80.2	80.2	186.5	187.9	187.8
1900	183.8	186.1	183.9	80.2	81.2	81.2	194.4	195.9	195.8
2000	187.9	190.3	188.1	81.0	82.0	82.0	202.5	204.1	204.0
SP1									
200	87.8	89.0	85.9	29.1	28.9	26.1	99.9	99.9	99.6
250	94.8	96.0	92.2	34.1	33.7	30.9	101.5	101.5	101.0
300	101.5	102.5	98.3	39.0	38.4	35.9	103.3	103.3	102.7
350	107.9	108.8	104.2	43.8	43.2	41.0	105.4	105.3	104.6
400	114.0	114.9	110.0	48.3	47.7	45.9	107.7	107.6	106.8
450	119.9	120.8	115.7	52.6	52.0	50.5	110.2	110.1	109.2
500	125.7	126.5	121.2	56.4	55.9	54.7	113.0	112.8	111.8
550	131.2	132.0	126.6	59.8	59.5	58.5	115.9	115.7	114.7
600	136.6	137.3	131.9	63.0	62.8	61.9	118.9	118.8	117.7

650	141.7	142.4	136.9	65.8	65.7	65.0	122.2	122.0	120.9
700	146.7	147.4	141.9	68.3	68.4	67.8	125.5	125.3	124.2
750	151.5	152.2	146.6	70.6	70.9	70.3	129.0	128.8	127.6
800	156.1	156.8	151.2	72.7	73.1	72.6	132.6	132.4	131.2
850	160.6	161.3	155.7	74.7	75.2	74.7	136.3	136.1	134.9
900	164.9	165.7	160.0	76.4	77.1	76.7	140.0	139.9	138.7
950	169.1	169.9	164.2	78.1	78.9	78.5	143.9	143.8	142.6
1000	173.1	174.0	168.3	79.6	80.5	80.2	147.8	147.8	146.5
1100	180.8	181.8	176.1	82.3	83.4	83.2	155.9	156.0	154.7
1200	188.1	189.2	183.4	84.7	86.0	85.7	164.3	164.5	163.1
1300	195.0	196.2	190.4	86.7	88.1	87.9	172.9	173.2	171.8
1400	201.4	202.8	197.0	88.4	90.0	89.9	181.6	182.1	180.7
1500	207.6	209.0	203.2	90.0	91.7	91.5	190.5	191.2	189.8
1600	213.5	215.0	209.2	91.3	93.1	93.0	199.6	200.4	199.0
1700	219.0	220.7	214.9	92.5	94.4	94.3	208.8	209.8	208.4
1800	224.3	226.1	220.3	93.5	95.5	95.4	218.1	219.3	217.9
1900	229.4	231.3	225.5	94.4	96.5	96.4	227.5	228.9	227.5
2000	234.3	236.3	230.4	95.3	97.4	97.3	237.0	238.6	237.2

SP2a

200	82.7	83.8	81.2	32.8	33.1	24.9	99.8	99.8	99.4
250	90.8	91.9	87.3	39.1	39.1	30.0	101.6	101.6	100.7
300	98.3	99.4	93.2	43.3	42.9	35.3	103.7	103.7	102.4
350	105.2	106.3	99.1	46.9	46.3	40.7	105.9	105.9	104.3
400	111.7	112.7	104.9	50.6	49.9	45.8	108.4	108.3	106.4
450	117.9	118.8	110.5	54.2	53.6	50.5	111.0	110.9	108.9
500	123.8	124.6	116.1	57.7	57.2	54.8	113.8	113.7	111.5
550	129.5	130.2	121.5	60.9	60.6	58.6	116.7	116.6	114.3
600	134.9	135.6	126.7	63.8	63.7	62.1	119.9	119.7	117.3
650	140.1	140.8	131.8	66.5	66.5	65.2	123.1	123.0	120.5
700	145.1	145.9	136.8	69.0	69.1	68.0	126.5	126.4	123.9
750	150.0	150.7	141.5	71.2	71.5	70.5	130.0	129.9	127.3
800	154.6	155.4	146.2	73.3	73.7	72.8	133.6	133.5	130.9
850	159.1	159.9	150.6	75.2	75.7	74.9	137.3	137.2	134.6
900	163.5	164.3	155.0	76.9	77.6	76.9	141.1	141.1	138.4
950	167.7	168.6	159.2	78.5	79.3	78.7	145.0	145.0	142.3
1000	171.7	172.7	163.3	80.0	80.9	80.4	149.0	149.0	146.3
1100	179.5	180.5	171.1	82.7	83.8	83.3	157.1	157.3	154.4
1200	186.8	187.9	178.4	85.0	86.3	85.9	165.5	165.8	162.9
1300	193.7	194.9	185.4	87.0	88.4	88.1	174.1	174.5	171.6
1400	200.2	201.5	192.0	88.8	90.3	90.0	182.9	183.4	180.5
1500	206.4	207.8	198.2	90.3	91.9	91.7	191.9	192.5	189.6
1600	212.2	213.8	204.2	91.6	93.3	93.1	201.0	201.8	198.8
1700	217.8	219.5	209.9	92.8	94.6	94.4	210.2	211.2	208.2
1800	223.2	224.9	215.3	93.8	95.7	95.5	219.5	220.7	217.7
1900	228.3	230.1	220.5	94.7	96.7	96.5	228.9	230.3	227.3
2000	233.1	235.1	225.5	95.5	97.5	97.4	238.5	240.0	237.0

SP2b

200	91.4	92.0	87.0	27.0	26.9	26.4	99.3	99.2	99.0
250	97.9	98.4	93.4	31.5	31.5	31.2	100.7	100.7	100.4
300	104.0	104.6	99.5	36.4	36.6	36.3	102.4	102.4	102.1
350	110.0	110.7	105.5	41.4	41.7	41.5	104.4	104.3	104.0
400	115.9	116.5	111.4	46.2	46.6	46.4	106.5	106.5	106.2
450	121.6	122.3	117.1	50.6	51.2	51.0	109.0	109.0	108.7
500	127.1	127.9	122.7	54.7	55.4	55.2	111.6	111.6	111.3
550	132.5	133.4	128.1	58.3	59.1	59.0	114.4	114.5	114.2
600	137.7	138.7	133.4	61.6	62.5	62.4	117.4	117.5	117.2
650	142.8	143.8	138.5	64.5	65.5	65.4	120.6	120.7	120.4
700	147.6	148.7	143.5	67.1	68.3	68.2	123.9	124.1	123.8
750	152.4	153.5	148.3	69.5	70.8	70.7	127.3	127.6	127.2
800	156.9	158.2	152.9	71.7	73.1	73.0	130.8	131.2	130.8
850	161.3	162.7	157.4	73.7	75.2	75.1	134.5	134.9	134.5
900	165.6	167.0	161.8	75.6	77.1	77.0	138.2	138.7	138.3
950	169.7	171.3	166.0	77.3	78.9	78.8	142.0	142.6	142.2
1000	173.7	175.3	170.1	78.8	80.5	80.5	145.9	146.6	146.2
1100	181.4	183.2	177.9	81.7	83.5	83.4	154.0	154.8	154.4
1200	188.6	190.5	185.2	84.1	86.0	85.9	162.2	163.2	162.9
1300	195.4	197.5	192.2	86.2	88.2	88.1	170.8	172.0	171.6
1400	201.9	204.1	198.8	88.0	90.1	90.0	179.5	180.9	180.5
1500	208.0	210.4	205.1	89.6	91.7	91.7	188.3	190.0	189.6
1600	213.8	216.3	211.0	90.9	93.2	93.1	197.4	199.2	198.8
1700	219.4	222.0	216.7	92.1	94.4	94.4	206.5	208.6	208.2
1800	224.7	227.5	222.2	93.2	95.6	95.5	215.8	218.1	217.7
1900	229.7	232.7	227.4	94.2	96.5	96.5	225.2	227.7	227.3
2000	234.6	237.6	232.3	95.0	97.4	97.4	234.6	237.4	237.0

SP3a

200	81.6	82.3	81.2	28.7	28.0	24.9	99.5	99.5	99.3
250	88.8	89.3	87.3	36.2	35.3	29.9	101.2	101.1	100.7
300	96.0	96.4	93.2	43.4	43.0	35.2	103.2	103.0	102.3
350	103.2	103.6	99.1	49.5	50.3	40.6	105.5	105.4	104.2
400	110.1	110.8	104.8	54.3	56.3	45.7	108.1	108.1	106.4
450	116.7	117.7	110.5	58.1	60.8	50.4	110.9	111.0	108.8
500	123.0	124.2	116.0	61.2	64.0	54.7	113.9	114.1	111.4
550	129.0	130.5	121.4	63.8	66.5	58.5	117.0	117.4	114.3
600	134.6	136.3	126.7	66.1	68.6	62.0	120.3	120.8	117.3
650	140.0	141.9	131.8	68.2	70.5	65.1	123.6	124.2	120.5
700	145.1	147.2	136.7	70.2	72.4	67.9	127.1	127.8	123.8
750	150.1	152.3	141.5	72.1	74.1	70.5	130.6	131.5	127.2
800	154.8	157.1	146.1	73.9	75.8	72.8	134.3	135.2	130.8
850	159.3	161.8	150.6	75.6	77.5	74.9	138.0	139.0	134.5
900	163.7	166.2	154.9	77.1	79.0	76.9	141.8	143.0	138.3
950	167.9	170.5	159.1	78.6	80.5	78.7	145.7	147.0	142.2
1000	171.9	174.7	163.2	80.0	81.9	80.3	149.7	151.0	146.2
1100	179.7	182.6	171.0	82.5	84.5	83.3	157.8	159.3	154.4
1200	187.0	190.1	178.3	84.7	86.8	85.9	166.2	167.9	162.8

1300	193.8	197.1	185.3	86.7	88.8	88.1	174.8	176.7	171.5
1400	200.3	203.8	191.9	88.4	90.6	90.0	183.5	185.7	180.4
1500	206.5	210.1	198.2	89.9	92.1	91.7	192.4	194.8	189.5
1600	212.3	216.1	204.1	91.2	93.5	93.1	201.5	204.1	198.8
1700	217.9	221.8	209.8	92.4	94.7	94.4	210.7	213.5	208.1
1800	223.2	227.2	215.3	93.4	95.8	95.5	220.0	223.0	217.6
1900	228.3	232.4	220.5	94.4	96.8	96.5	229.4	232.6	227.2
2000	233.1	237.4	225.4	95.2	97.6	97.4	238.8	242.4	236.9

SP3b

200	90.7	91.2	85.8	27.7	27.1	26.4	99.2	99.2	99.0
250	97.3	97.7	92.2	32.2	31.7	31.2	100.7	100.7	100.4
300	103.6	104.0	98.4	37.0	36.6	36.3	102.5	102.4	102.1
350	109.7	110.0	104.3	42.0	41.7	41.4	104.4	104.3	104.0
400	115.6	115.9	110.2	46.7	46.6	46.4	106.7	106.5	106.2
450	121.4	121.6	115.9	51.1	51.2	51.0	109.1	109.0	108.7
500	127.0	127.2	121.5	55.1	55.3	55.2	111.8	111.6	111.3
550	132.4	132.7	127.0	58.7	59.1	58.9	114.6	114.5	114.2
600	137.7	138.0	132.2	62.0	62.4	62.3	117.6	117.5	117.2
650	142.7	143.1	137.4	64.9	65.5	65.4	120.8	120.7	120.4
700	147.7	148.0	142.3	67.5	68.2	68.2	124.1	124.1	123.8
750	152.4	152.8	147.1	69.9	70.8	70.7	127.5	127.6	127.2
800	157.0	157.5	151.7	72.0	73.0	73.0	131.1	131.2	130.8
850	161.4	162.0	156.2	74.0	75.1	75.1	134.7	134.9	134.5
900	165.7	166.3	160.6	75.8	77.1	77.0	138.5	138.7	138.3
950	169.8	170.5	164.8	77.5	78.9	78.8	142.3	142.6	142.2
1000	173.8	174.6	168.9	79.1	80.5	80.5	146.2	146.5	146.2
1100	181.5	182.4	176.7	81.8	83.4	83.4	154.3	154.8	154.4
1200	188.7	189.8	184.1	84.2	86.0	85.9	162.6	163.2	162.9
1300	195.6	196.8	191.0	86.3	88.2	88.1	171.1	171.9	171.6
1400	202.0	203.4	197.6	88.1	90.1	90.0	179.8	180.8	180.5
1500	208.1	209.7	203.9	89.6	91.7	91.7	188.7	189.9	189.6
1600	214.0	215.6	209.9	91.0	93.2	93.1	197.8	199.2	198.8
1700	219.5	221.3	215.5	92.2	94.4	94.4	206.9	208.6	208.2
1800	224.8	226.7	221.0	93.2	95.6	95.5	216.2	218.1	217.7
1900	229.9	231.9	226.2	94.2	96.5	96.5	225.6	227.7	227.3
2000	234.7	236.9	231.1	95.0	97.4	97.4	235.0	237.4	237.0

SP4

200	91.2	91.9	89.2	27.8	27.3	25.6	99.2	99.2	98.9
250	97.8	98.4	95.4	32.0	31.5	30.2	100.7	100.6	100.3
300	104.1	104.5	101.4	36.8	36.2	35.3	102.4	102.3	101.9
350	110.1	110.5	107.2	41.7	41.1	40.5	104.4	104.2	103.8
400	116.0	116.3	112.9	46.5	46.0	45.5	106.6	106.4	105.9
450	121.8	122.0	118.6	51.0	50.5	50.2	109.0	108.8	108.3
500	127.4	127.5	124.1	55.1	54.7	54.4	111.7	111.5	111.0
550	132.8	132.9	129.4	58.8	58.5	58.3	114.5	114.3	113.8
600	138.0	138.2	134.7	62.1	61.9	61.7	117.5	117.3	116.8
650	143.1	143.2	139.7	65.1	65.0	64.9	120.7	120.5	119.9

700	148.1	148.2	144.6	67.7	67.8	67.7	124.0	123.8	123.3
750	152.8	152.9	149.4	70.1	70.4	70.3	127.5	127.3	126.7
800	157.4	157.6	154.0	72.4	72.8	72.7	131.1	130.8	130.3
850	161.9	162.0	158.5	74.4	74.9	74.8	134.7	134.5	134.0
900	166.2	166.4	162.8	76.2	76.9	76.8	138.5	138.3	137.8
950	170.3	170.6	167.0	77.9	78.7	78.7	142.3	142.2	141.6
1000	174.4	174.7	171.1	79.5	80.4	80.3	146.3	146.2	145.6
1100	182.1	182.5	178.9	82.3	83.4	83.4	154.4	154.4	153.8
1200	189.3	189.8	186.3	84.7	86.0	86.0	162.7	162.9	162.3
1300	196.2	196.8	193.2	86.7	88.2	88.2	171.3	171.6	171.0
1400	202.7	203.4	199.8	88.5	90.2	90.1	180.1	180.5	179.9
1500	208.9	209.7	206.1	90.1	91.8	91.8	189.0	189.6	189.0
1600	214.7	215.7	212.1	91.4	93.3	93.3	198.1	198.9	198.3
1700	220.3	221.4	217.8	92.6	94.6	94.5	207.3	208.3	207.7
1800	225.6	226.8	223.2	93.6	95.7	95.7	216.6	217.8	217.2
1900	230.7	232.0	228.4	94.5	96.7	96.7	226.0	227.4	226.8
2000	235.6	237.0	233.4	95.4	97.6	97.5	235.5	237.1	236.5

SP_{cpt}

200	84.6	85.5	83.3	23.4	23.1	22.8	95.9	95.9	95.8
250	90.3	91.0	88.9	27.7	27.2	27.1	97.2	97.1	97.0
300	95.8	96.4	94.2	32.5	32.0	31.9	98.7	98.6	98.5
350	101.1	101.7	99.5	37.3	36.9	36.8	100.4	100.3	100.2
400	106.4	107.0	104.8	42.0	41.6	41.6	102.4	102.3	102.2
450	111.6	112.1	109.9	46.4	46.0	46.0	104.6	104.5	104.3
500	116.7	117.2	115.0	50.4	50.1	50.1	107.0	106.9	106.7
550	121.7	122.1	119.9	54.0	53.8	53.7	109.6	109.5	109.3
600	126.5	127.0	124.7	57.2	57.1	57.1	112.4	112.3	112.1
650	131.2	131.6	129.4	60.1	60.1	60.1	115.4	115.2	115.0
700	135.8	136.2	134.0	62.7	62.8	62.8	118.4	118.3	118.1
750	140.2	140.6	138.4	65.1	65.3	65.3	121.6	121.5	121.3
800	144.5	144.9	142.7	67.3	67.6	67.6	124.9	124.8	124.6
850	148.6	149.1	146.8	69.3	69.7	69.7	128.4	128.2	128.1
900	152.6	153.1	150.9	71.1	71.6	71.6	131.9	131.8	131.6
950	156.5	157.0	154.8	72.8	73.4	73.4	135.5	135.4	135.2
1000	160.3	160.8	158.6	74.4	75.0	75.0	139.1	139.1	138.9
1100	167.5	168.1	165.9	77.2	77.9	77.9	146.7	146.7	146.6
1200	174.3	175.0	172.8	79.6	80.5	80.4	154.6	154.7	154.5
1300	180.8	181.5	179.3	81.6	82.6	82.6	162.6	162.8	162.7
1400	186.9	187.7	185.5	83.4	84.5	84.5	170.9	171.2	171.0
1500	192.7	193.6	191.4	85.0	86.2	86.1	179.3	179.7	179.6
1600	198.2	199.2	197.0	86.3	87.6	87.6	187.9	188.4	188.3
1700	203.5	204.6	202.4	87.5	88.8	88.8	196.6	197.2	197.1
1800	208.5	209.7	207.5	88.5	89.9	89.9	205.4	206.2	206.0
1900	213.3	214.6	212.4	89.5	90.9	90.9	214.3	215.2	215.1
2000	217.9	219.3	217.0	90.3	91.8	91.8	223.2	224.3	224.2

^a The zero of energy is set equal to the potential energy of the global minimum.

^b Calculated using the lowest-energy conformer.

6. Location of generalized transition state at different temperatures

Table S9 Location of generalized transition state along different temperatures.

T (K)	R1	R2a	R2b	R3a	R3b	R4	<i>Rcpt</i>
200	-0.1676	0.0189	0.0055	0.0141	-0.0036	0.011	-0.0195
250	-0.1669	0.0195	0.0052	0.0136	-0.0036	0.0104	-0.02
300	-0.1664	0.0204	0.0051	0.0131	-0.0036	0.01	-0.0206
350	-0.166	0.0213	0.0049	0.0128	-0.0036	0.0095	-0.0213
400	-0.1658	0.0224	0.0048	0.0126	-0.0035	0.0091	-0.022
450	-0.1656	0.0237	0.0047	0.0124	-0.0035	0.0087	-0.0231
500	-0.1656	0.0252	0.0046	0.0124	-0.0035	0.0083	-0.0246
550	-0.1655	0.0268	0.0045	0.0124	-0.0034	0.008	-0.0261
600	-0.1656	0.0284	0.0045	0.0124	-0.0034	0.0078	-0.0277
650	-0.1656	0.03	0.0044	0.0125	-0.0034	0.0075	-0.0294
700	-0.1657	0.0317	0.0044	0.0126	-0.0033	0.0073	-0.0311
750	-0.1658	0.0334	0.0043	0.0127	-0.0033	0.007	-0.0328
800	-0.1659	0.0351	0.0043	0.0128	-0.0033	0.0068	-0.0346
850	-0.166	0.0369	0.0042	0.013	-0.0032	0.0067	-0.0363
900	-0.1661	0.0386	0.0042	0.0131	-0.0032	0.0065	-0.0381
950	-0.1662	0.0404	0.0041	0.0133	-0.0032	0.0063	-0.0399
1000	-0.1664	0.0421	0.0041	0.0134	-0.0031	0.0062	-0.0417
1100	-0.1666	0.0456	0.004	0.0138	-0.0031	0.0059	-0.1714
1200	-0.1668	0.0491	0.004	0.0141	-0.003	0.0057	-0.1728
1300	-0.167	0.0525	0.0039	0.0145	-0.003	0.0054	-0.1739
1400	-0.1672	0.056	0.0039	0.0148	-0.003	0.0052	-0.175
1500	-0.1674	0.0593	0.0038	0.0151	-0.0029	0.005	-0.1759
1600	-0.1676	0.2174	0.0038	0.0155	-0.0029	0.0049	-0.1767
1700	-0.1678	0.2184	0.0037	0.0158	-0.0028	0.0047	-0.1775
1800	-0.1679	0.2193	0.0037	0.0161	-0.0028	0.0046	-0.1781
1900	-0.1681	0.2201	0.0037	0.0164	-0.0028	0.0044	-0.1787

2000	-0.1682	0.2208	0.0036	0.0166	-0.0027	0.0043	-0.1793
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7. Transmission coefficients

Table S10 Canonical recrossing coefficients at different temperatures.

T (K)	R1	R2a	R2b	R3a	R3b	R4	<i>Rcpt</i>
200	0.203	0.848	0.739	0.875	0.815	0.990	0.873
250	0.244	0.868	0.758	0.897	0.817	0.993	0.890
300	0.272	0.880	0.772	0.911	0.820	0.996	0.899
350	0.290	0.887	0.782	0.921	0.823	0.997	0.905
400	0.301	0.890	0.791	0.927	0.827	0.998	0.909
450	0.307	0.898	0.798	0.932	0.831	0.998	0.916
500	0.309	0.897	0.805	0.935	0.834	0.999	0.916
550	0.310	0.896	0.810	0.937	0.838	0.999	0.916
600	0.308	0.894	0.815	0.938	0.841	0.999	0.915
650	0.306	0.891	0.819	0.939	0.844	1.000	0.913
700	0.303	0.888	0.823	0.940	0.847	1.000	0.912
750	0.300	0.884	0.826	0.940	0.850	1.000	0.910
800	0.296	0.880	0.830	0.941	0.853	1.000	0.908
850	0.293	0.876	0.833	0.941	0.855	1.000	0.905
900	0.289	0.872	0.835	0.941	0.858	1.000	0.903
950	0.286	0.868	0.838	0.940	0.860	1.000	0.901
1000	0.282	0.864	0.840	0.940	0.862	1.000	0.898
1100	0.275	0.855	0.845	0.940	0.866	1.000	0.837
1200	0.269	0.846	0.849	0.939	0.870	1.000	0.770
1300	0.263	0.837	0.852	0.938	0.873	1.000	0.715
1400	0.258	0.828	0.856	0.937	0.876	1.000	0.670
1500	0.254	0.819	0.859	0.937	0.879	1.000	0.632
1600	0.249	0.749	0.861	0.936	0.882	1.000	0.601
1700	0.245	0.684	0.864	0.935	0.884	1.000	0.573
1800	0.242	0.631	0.866	0.935	0.887	1.000	0.549
1900	0.239	0.586	0.869	0.934	0.889	1.000	0.529

2000	0.236	0.548	0.871	0.933	0.891	1.000	0.511
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Table S11 Tunneling transmission coefficients calculated using the multi-dimensional small-curvature tunneling (SCT) approximation and zero-curvature tunneling (ZCT) approximation, as well as one-dimensional Eckart tunneling (ET) approximation.

T (K)	R1	R2a	R2b	R3a	R3b	R4	<i>Rc_{pt}</i>
SCT							
200	24.98	1127.30	477.35	195.18	575.05	6.70	631.13
250	7.55	140.26	62.30	46.56	66.90	3.73	70.94
300	4.05	38.72	19.47	18.58	19.80	2.62	20.49
350	2.80	16.55	9.38	9.92	9.29	2.08	9.49
400	2.20	9.18	5.74	6.34	5.62	1.77	5.70
450	1.87	6.00	4.06	4.56	3.95	1.58	4.00
500	1.66	4.38	3.15	3.54	3.06	1.46	3.09
550	1.52	3.45	2.60	2.92	2.52	1.37	2.55
600	1.43	2.86	2.24	2.50	2.18	1.31	2.21
650	1.35	2.46	2.00	2.21	1.94	1.26	1.97
700	1.30	2.19	1.82	2.00	1.77	1.22	1.79
750	1.26	1.99	1.69	1.84	1.64	1.19	1.67
800	1.22	1.83	1.58	1.72	1.54	1.16	1.57
850	1.19	1.71	1.50	1.62	1.47	1.14	1.49
900	1.17	1.62	1.44	1.54	1.41	1.13	1.43
950	1.15	1.54	1.39	1.48	1.36	1.11	1.38
1000	1.14	1.48	1.34	1.43	1.31	1.10	1.33
1100	1.11	1.38	1.28	1.34	1.25	1.08	1.27
1200	1.09	1.32	1.23	1.28	1.20	1.07	1.22
1300	1.08	1.26	1.19	1.24	1.17	1.06	1.19
1400	1.07	1.22	1.16	1.20	1.14	1.05	1.16
1500	1.06	1.19	1.14	1.17	1.12	1.04	1.14

1600	1.05	1.17	1.12	1.15	1.11	1.04	1.12
1700	1.05	1.15	1.11	1.13	1.09	1.03	1.11
1800	1.04	1.13	1.09	1.12	1.08	1.03	1.09
1900	1.04	1.12	1.08	1.11	1.07	1.03	1.08
2000	1.03	1.10	1.07	1.10	1.06	1.02	1.08

ZCT

200	4.26	139.29	51.10	89.25	37.10	4.03	39.63
250	2.45	28.13	14.30	24.03	10.09	2.52	10.48
300	1.85	11.17	6.85	10.61	4.98	1.92	5.13
350	1.57	6.22	4.29	6.17	3.25	1.62	3.34
400	1.41	4.18	3.12	4.22	2.46	1.45	2.53
450	1.31	3.16	2.49	3.21	2.03	1.34	2.09
500	1.25	2.57	2.11	2.62	1.76	1.27	1.82
550	1.20	2.20	1.86	2.24	1.59	1.22	1.64
600	1.16	1.95	1.69	1.99	1.47	1.18	1.52
650	1.14	1.77	1.57	1.81	1.39	1.15	1.43
700	1.12	1.64	1.48	1.67	1.32	1.13	1.36
750	1.10	1.54	1.40	1.57	1.27	1.11	1.31
800	1.09	1.47	1.35	1.49	1.23	1.10	1.27
850	1.08	1.41	1.30	1.42	1.20	1.09	1.23
900	1.07	1.36	1.27	1.37	1.17	1.08	1.20
950	1.06	1.32	1.24	1.33	1.15	1.07	1.18
1000	1.06	1.28	1.21	1.29	1.14	1.06	1.16
1100	1.05	1.23	1.17	1.24	1.11	1.05	1.13
1200	1.04	1.19	1.14	1.20	1.09	1.04	1.11
1300	1.03	1.16	1.12	1.17	1.07	1.03	1.09
1400	1.03	1.14	1.10	1.14	1.06	1.03	1.08
1500	1.02	1.12	1.09	1.12	1.05	1.03	1.07
1600	1.02	1.10	1.08	1.11	1.04	1.02	1.06

1700	1.02	1.09	1.07	1.09	1.04	1.02	1.05
1800	1.02	1.08	1.06	1.08	1.03	1.02	1.05
1900	1.02	1.07	1.05	1.07	1.03	1.01	1.04
2000	1.01	1.06	1.05	1.07	1.02	1.01	1.04

ET

200	88.73	488.44	1174.33	60.46	1255.86	7.54	1093.44
250	17.91	70.38	105.42	17.67	102.91	4.22	93.99
300	7.29	21.39	25.48	8.48	24.46	3.01	23.08
350	4.23	9.99	10.61	5.21	10.06	2.39	9.66
400	2.99	5.97	5.99	3.70	5.71	2.03	5.53
450	2.36	4.15	4.06	2.89	3.88	1.80	3.80
500	1.99	3.19	3.08	2.41	2.96	1.65	2.91
550	1.76	2.62	2.51	2.10	2.43	1.57	2.40
600	1.60	2.25	2.16	1.89	2.10	1.46	2.07
650	1.49	2.00	1.92	1.76	1.87	1.43	1.85
700	1.41	1.82	1.75	1.63	1.71	1.35	1.69
750	1.34	1.68	1.62	1.53	1.59	1.31	1.58
800	1.30	1.58	1.53	1.46	1.50	1.29	1.49
850	1.26	1.50	1.45	1.40	1.43	1.25	1.42
900	1.22	1.43	1.39	1.36	1.37	1.23	1.37
950	1.20	1.38	1.34	1.32	1.33	1.22	1.32
1000	1.18	1.34	1.30	1.29	1.29	1.20	1.28
1100	1.14	1.27	1.24	1.24	1.23	1.17	1.23
1200	1.12	1.22	1.20	1.20	1.19	1.14	1.18
1300	1.10	1.19	1.16	1.18	1.16	1.15	1.15
1400	1.08	1.16	1.14	1.15	1.13	1.11	1.13
1500	1.07	1.13	1.12	1.13	1.11	1.11	1.11
1600	1.06	1.12	1.10	1.11	1.10	1.11	1.10
1700	1.05	1.10	1.09	1.10	1.08	1.09	1.08

1800	1.05	1.09	1.08	1.09	1.07	1.08	1.07
1900	1.04	1.08	1.07	1.08	1.07	1.07	1.06
2000	1.04	1.07	1.06	1.07	1.06	1.07	1.06

8. Changes of vibrational frequencies along the reaction coordinate

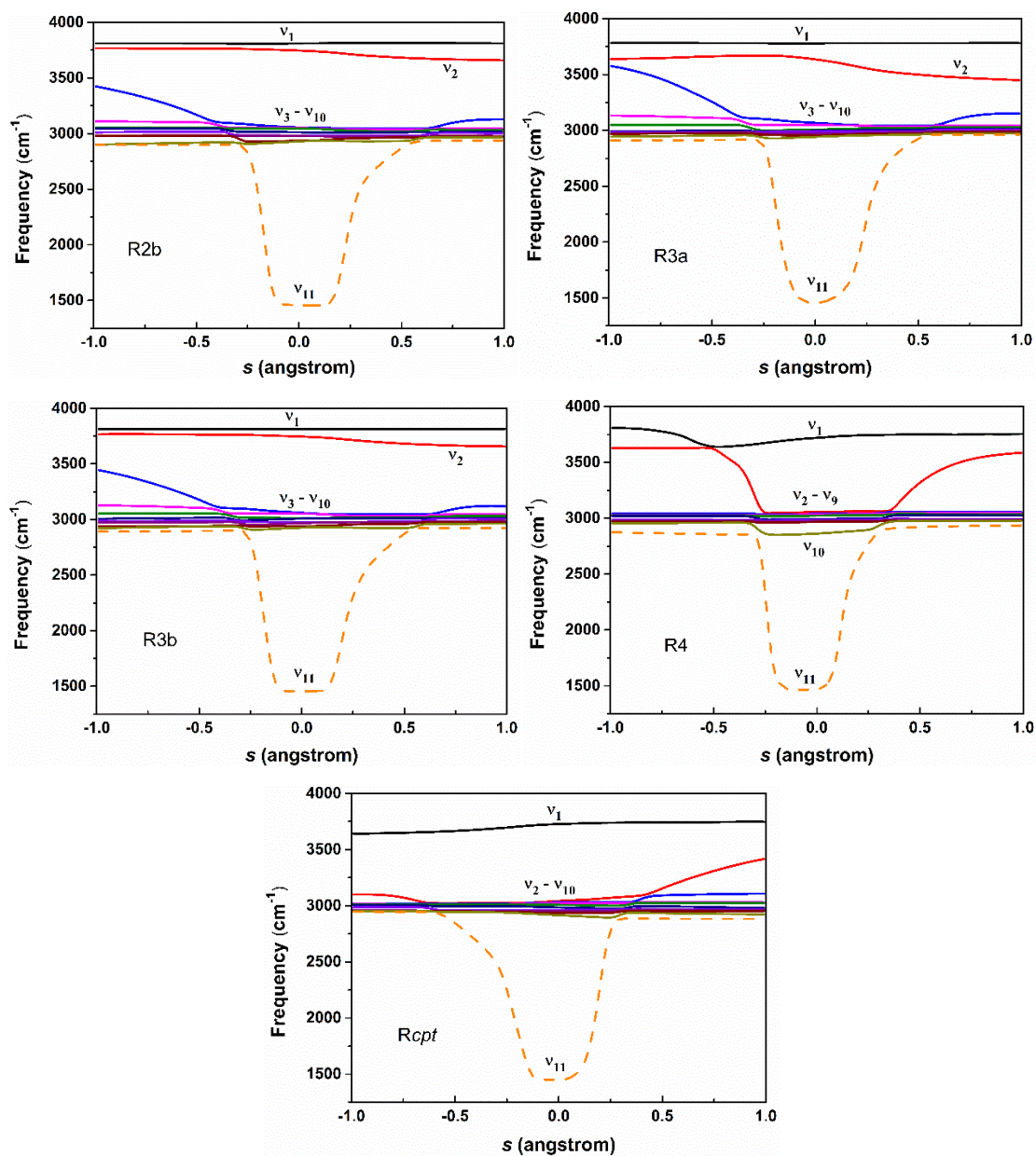


Figure S1 The eleven highest vibrational frequencies for R2b, R3a, R3b, R4 and Rcpt as functions of the reaction coordinate (s). The saddle points are located at $s = 0$.

9. Vibrationally adiabatic ground energy along MEPs

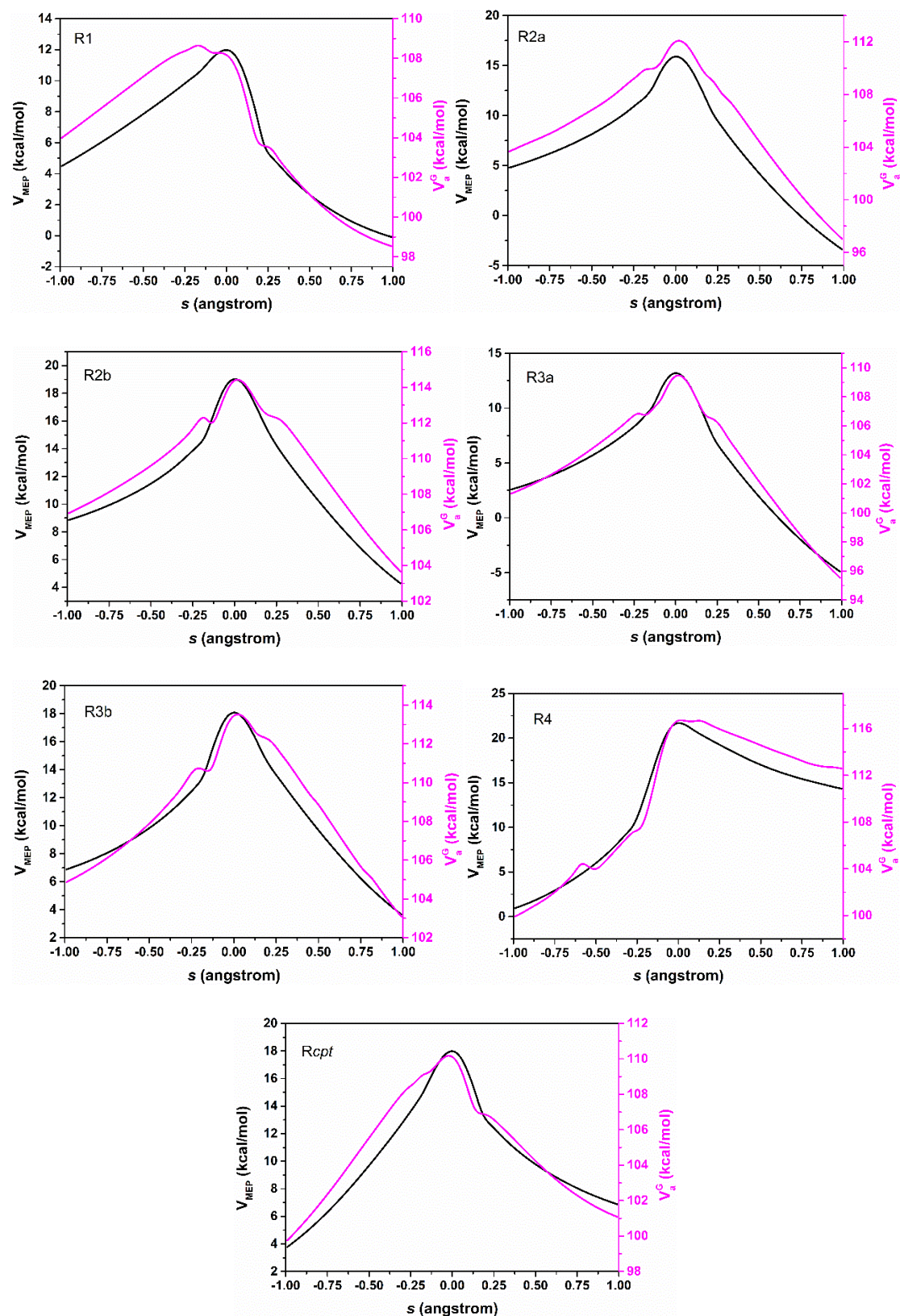


Fig. S2 The potential energy (V_{MEP}) and vibrationally adiabatic ground energy (V_a^G) with respect to the reaction coordinate (s).

10. Tabulated rate constants using different methods

From Fig. S3, the SS-QH-TST method is observed to significantly underestimate rate constants as compared with MS-T-CVT/SCT method except for R1. The ratios of $k^{\text{MS-T-CVT/SCT}}$ to $k^{\text{SS-QH-TST}}$ lie in the range of 0.8 – 1486 at atmospheric conditions (200 – 500 K) and are within 0.8 – 22.7 at typical combustion conditions (500 – 2000 K). This significant deviation at low temperatures is mainly caused by the multi-dimensional tunneling effect and the key factor is superseded by the anharmonicity effect at high temperatures, while the variational effect is moderate over the entire temperature range. The ratios of $k^{\text{MS-T-TST/Eckart}}$ to $k^{\text{MS-T-CVT/SCT}}$ lie in the range of 0.35 – 17.6, and the largest discrepancy is observed in the case of α -carbon site (R1) caused by the strong variational effect. The ratios of $k^{\text{MS-T-TST/Eckart}}$ to $k^{\text{MS-T-CVT/SCT}}$ lie in the range of 0.35 – 17.6. To facilitate usage for various purposes, numerical values in tabular form calculated using three different methods are also provided in Table S12.

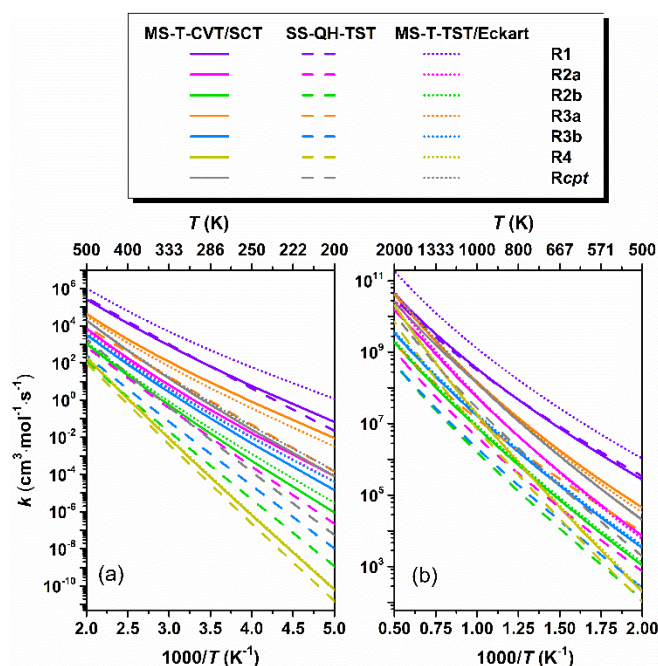


Fig. S3 The site-specific rate constants per hydrogen atom of H-atom abstraction reactions from cyclopentanol and cyclopentane by HO_2 calculated by MS-T-CVT/SCT (solid lines), MS-T-TST/Eckart (dotted lines) and SS-QH-TST (dashed lines) methods over the temperature range of (a) 200 – 500 K and (b) 500–2000 K.

Table S12 The site-specific rate constants per hydrogen atom of H-atom abstraction reactions from cyclopentanol and cyclopentane by HO₂ radical calculated using MS-T-CVT/SCT method.

T (K)	R1	R2a	R2b	R3a	R3b	R4	<i>R_{cpt}</i>
Forward reactions							
200	6.71E-02	8.22E-05	8.92E-07	9.03E-03	1.45E-05	6.26E-11	8.14E-05
250	5.68E+00	1.67E-02	5.38E-04	8.12E-01	4.69E-03	6.30E-07	2.53E-02
300	1.48E+02	8.05E-01	5.01E-02	2.04E+01	2.98E-01	3.39E-04	1.61E+00
350	1.82E+03	1.62E+01	1.50E+00	2.46E+02	6.96E+00	3.39E-02	3.78E+01
400	1.34E+04	1.81E+02	2.14E+01	1.87E+03	8.30E+01	1.17E+00	4.62E+02
450	6.84E+04	1.33E+03	1.82E+02	1.02E+04	6.20E+02	1.95E+01	3.59E+03
500	2.67E+05	7.15E+03	1.07E+03	4.42E+04	3.30E+03	1.96E+02	1.98E+04
550	8.58E+05	3.02E+04	4.74E+03	1.58E+05	1.36E+04	1.36E+03	8.41E+04
600	2.35E+06	1.06E+05	1.70E+04	4.81E+05	4.58E+04	7.04E+03	2.94E+05
650	5.69E+06	3.17E+05	5.17E+04	1.30E+06	1.32E+05	2.92E+04	8.76E+05
700	1.24E+07	8.43E+05	1.37E+05	3.16E+06	3.35E+05	1.02E+05	2.30E+06
750	2.49E+07	2.02E+06	3.23E+05	7.02E+06	7.62E+05	3.06E+05	5.43E+06
800	4.68E+07	4.43E+06	6.98E+05	1.45E+07	1.61E+06	8.15E+05	1.18E+07
850	8.26E+07	9.05E+06	1.39E+06	2.80E+07	3.13E+06	1.97E+06	2.36E+07
900	1.39E+08	1.73E+07	2.61E+06	5.12E+07	5.73E+06	4.37E+06	4.45E+07
950	2.23E+08	3.14E+07	4.61E+06	8.91E+07	9.93E+06	9.04E+06	7.94E+07
1000	3.46E+08	5.44E+07	7.74E+06	1.48E+08	1.64E+07	1.75E+07	1.35E+08
1100	7.57E+08	1.44E+08	1.95E+07	3.70E+08	4.02E+07	5.68E+07	3.27E+08
1200	1.49E+09	3.34E+08	4.29E+07	8.17E+08	8.65E+07	1.56E+08	6.86E+08
1300	2.69E+09	7.01E+08	8.52E+07	1.63E+09	1.68E+08	3.73E+08	1.31E+09
1400	4.56E+09	1.34E+09	1.55E+08	3.03E+09	3.02E+08	8.07E+08	2.32E+09
1500	7.29E+09	2.39E+09	2.64E+08	5.26E+09	5.06E+08	1.60E+09	3.85E+09
1600	1.12E+10	3.74E+09	4.24E+08	8.64E+09	8.05E+08	2.94E+09	6.08E+09
1700	1.65E+10	5.59E+09	6.50E+08	1.35E+10	1.22E+09	5.13E+09	9.20E+09
1800	2.34E+10	8.05E+09	9.53E+08	2.04E+10	1.78E+09	8.44E+09	1.34E+10

1900	3.24E+10	1.12E+10	1.36E+09	2.97E+10	2.50E+09	1.33E+10	1.89E+10
2000	4.36E+10	1.53E+10	1.87E+09	4.21E+10	3.43E+09	2.03E+10	2.61E+10

Reverse reactions

200	8.40E+04	1.36E+06	2.19E+05	2.81E+07	1.98E+05	6.60E+08	1.30E+06
250	4.39E+05	2.38E+06	6.89E+05	3.41E+07	6.14E+05	1.17E+09	4.26E+06
300	1.75E+06	4.64E+06	1.86E+06	4.69E+07	1.70E+06	1.99E+09	1.25E+07
350	5.47E+06	9.17E+06	4.33E+06	6.93E+07	4.10E+06	3.24E+09	3.17E+07
400	1.42E+07	1.76E+07	8.87E+06	1.07E+08	8.72E+06	5.07E+09	7.14E+07
450	3.21E+07	3.24E+07	1.64E+07	1.66E+08	1.68E+07	7.64E+09	1.47E+08
500	6.45E+07	5.67E+07	2.82E+07	2.60E+08	2.98E+07	1.12E+10	2.75E+08
550	1.20E+08	9.48E+07	4.53E+07	3.98E+08	4.93E+07	1.59E+10	4.78E+08
600	2.06E+08	1.52E+08	6.91E+07	5.98E+08	7.77E+07	2.20E+10	7.89E+08
650	3.36E+08	2.34E+08	1.01E+08	8.83E+08	1.17E+08	2.98E+10	1.24E+09
700	5.21E+08	3.51E+08	1.43E+08	1.27E+09	1.69E+08	3.97E+10	1.87E+09
750	7.77E+08	5.10E+08	1.95E+08	1.78E+09	2.35E+08	5.19E+10	2.73E+09
800	1.12E+09	7.17E+08	2.61E+08	2.46E+09	3.21E+08	6.67E+10	3.87E+09
850	1.57E+09	9.92E+08	3.40E+08	3.33E+09	4.27E+08	8.47E+10	5.31E+09
900	2.14E+09	1.34E+09	4.34E+08	4.42E+09	5.54E+08	1.06E+11	7.16E+09
950	2.86E+09	1.77E+09	5.45E+08	5.78E+09	7.07E+08	1.31E+11	9.43E+09
1000	3.75E+09	2.32E+09	6.72E+08	7.42E+09	8.87E+08	1.60E+11	1.22E+10
1100	6.13E+09	3.75E+09	9.89E+08	1.18E+10	1.34E+09	2.33E+11	1.84E+10
1200	9.43E+09	5.76E+09	1.39E+09	1.79E+10	1.92E+09	3.27E+11	2.59E+10
1300	1.39E+10	8.53E+09	1.89E+09	2.59E+10	2.66E+09	4.45E+11	3.53E+10
1400	1.97E+10	1.21E+10	2.48E+09	3.65E+10	3.56E+09	5.93E+11	4.68E+10
1500	2.70E+10	1.67E+10	3.18E+09	4.99E+10	4.62E+09	7.71E+11	6.05E+10
1600	3.62E+10	2.07E+10	3.99E+09	6.66E+10	5.87E+09	9.81E+11	7.66E+10
1700	4.73E+10	2.53E+10	4.90E+09	8.67E+10	7.28E+09	1.24E+12	9.55E+10
1800	6.05E+10	3.05E+10	5.92E+09	1.11E+11	8.93E+09	1.52E+12	1.17E+11
1900	7.61E+10	3.63E+10	7.08E+09	1.39E+11	1.07E+10	1.86E+12	1.42E+11

2000	9.43E+10	4.28E+10	8.34E+09	1.73E+11	1.28E+10	2.24E+12	1.69E+11
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Table S13 The site-specific rate constants per hydrogen atom of H-atom abstraction reactions from cyclopentanol and cyclopentane by HO₂ radical calculated using MS-LH-CVT/SCT method.

T (K)	R1	R2a	R2b	R3a	R3b	R4	<i>R_{cpt}</i>
Forward reactions							
200	9.60E-02	1.10E-04	1.08E-06	1.13E-02	1.68E-05	7.46E-11	1.31E-04
250	7.93E+00	2.21E-02	6.18E-04	9.69E-01	5.14E-03	7.17E-07	4.02E-02
300	2.01E+02	1.05E+00	5.52E-02	2.30E+01	3.11E-01	3.69E-04	2.51E+00
350	2.39E+03	2.05E+01	1.60E+00	2.64E+02	6.91E+00	3.52E-02	5.79E+01
400	1.69E+04	2.23E+02	2.22E+01	1.94E+03	7.89E+01	1.16E+00	6.95E+02
450	8.35E+04	1.59E+03	1.85E+02	1.05E+04	5.67E+02	1.86E+01	5.32E+03
500	3.15E+05	8.28E+03	1.06E+03	4.50E+04	2.91E+03	1.79E+02	2.89E+04
550	9.76E+05	3.39E+04	4.66E+03	1.61E+05	1.16E+04	1.19E+03	1.21E+05
600	2.59E+06	1.15E+05	1.65E+04	4.99E+05	3.81E+04	5.96E+03	4.18E+05
650	6.06E+06	3.35E+05	4.96E+04	1.37E+06	1.07E+05	2.39E+04	1.23E+06
700	1.28E+07	8.67E+05	1.30E+05	3.39E+06	2.66E+05	8.04E+04	3.21E+06
750	2.51E+07	2.03E+06	3.05E+05	7.67E+06	5.94E+05	2.35E+05	7.51E+06
800	4.59E+07	4.34E+06	6.56E+05	1.61E+07	1.23E+06	6.10E+05	1.62E+07
850	7.93E+07	8.69E+06	1.31E+06	3.18E+07	2.37E+06	1.44E+06	3.23E+07
900	1.30E+08	1.63E+07	2.43E+06	5.92E+07	4.28E+06	3.12E+06	6.07E+07
950	2.06E+08	2.90E+07	4.30E+06	1.05E+08	7.34E+06	6.33E+06	1.08E+08
1000	3.13E+08	4.95E+07	7.22E+06	1.78E+08	1.20E+07	1.20E+07	1.83E+08
1100	6.66E+08	1.28E+08	1.82E+07	4.57E+08	2.90E+07	3.78E+07	4.43E+08
1200	1.28E+09	2.89E+08	4.03E+07	1.04E+09	6.19E+07	1.01E+08	9.32E+08
1300	2.27E+09	5.95E+08	8.06E+07	2.14E+09	1.20E+08	2.37E+08	1.78E+09
1400	3.79E+09	1.12E+09	1.48E+08	4.10E+09	2.15E+08	5.05E+08	3.18E+09
1500	5.98E+09	1.98E+09	2.55E+08	7.33E+09	3.61E+08	9.88E+08	5.34E+09
1600	9.10E+09	3.07E+09	4.14E+08	1.24E+10	5.76E+08	1.80E+09	8.51E+09

1700	1.33E+10	4.56E+09	6.43E+08	1.99E+10	8.75E+08	3.12E+09	1.30E+10
1800	1.88E+10	6.54E+09	9.57E+08	3.08E+10	1.29E+09	5.12E+09	1.93E+10
1900	2.60E+10	9.11E+09	1.38E+09	4.61E+10	1.83E+09	8.07E+09	2.75E+10
2000	3.50E+10	1.24E+10	1.93E+09	6.68E+10	2.53E+09	1.23E+10	3.84E+10

Reverse reactions

200	1.20E+05	1.82E+06	2.65E+05	3.52E+07	2.29E+05	7.87E+08	2.09E+06
250	6.13E+05	3.15E+06	7.91E+05	4.07E+07	6.73E+05	1.34E+09	6.76E+06
300	2.36E+06	6.05E+06	2.05E+06	5.30E+07	1.77E+06	2.16E+09	1.95E+07
350	7.18E+06	1.16E+07	4.61E+06	7.45E+07	4.07E+06	3.36E+09	4.86E+07
400	1.80E+07	2.17E+07	9.21E+06	1.11E+08	8.29E+06	5.04E+09	1.07E+08
450	3.91E+07	3.87E+07	1.67E+07	1.71E+08	1.53E+07	7.27E+09	2.17E+08
500	7.60E+07	6.56E+07	2.80E+07	2.64E+08	2.62E+07	1.02E+10	4.01E+08
550	1.36E+08	1.06E+08	4.45E+07	4.07E+08	4.22E+07	1.39E+10	6.88E+08
600	2.27E+08	1.65E+08	6.70E+07	6.20E+08	6.46E+07	1.86E+10	1.12E+09
650	3.58E+08	2.48E+08	9.72E+07	9.29E+08	9.46E+07	2.44E+10	1.74E+09
700	5.38E+08	3.61E+08	1.36E+08	1.36E+09	1.34E+08	3.14E+10	2.61E+09
750	7.83E+08	5.11E+08	1.84E+08	1.95E+09	1.83E+08	3.99E+10	3.77E+09
800	1.10E+09	7.03E+08	2.45E+08	2.74E+09	2.46E+08	4.99E+10	5.32E+09
850	1.51E+09	9.52E+08	3.19E+08	3.78E+09	3.23E+08	6.19E+10	7.27E+09
900	2.01E+09	1.26E+09	4.04E+08	5.11E+09	4.14E+08	7.55E+10	9.76E+09
950	2.64E+09	1.64E+09	5.08E+08	6.81E+09	5.22E+08	9.17E+10	1.28E+10
1000	3.39E+09	2.10E+09	6.26E+08	8.90E+09	6.47E+08	1.09E+11	1.65E+10
1100	5.39E+09	3.33E+09	9.24E+08	1.46E+10	9.66E+08	1.55E+11	2.49E+10
1200	8.12E+09	4.98E+09	1.31E+09	2.27E+10	1.38E+09	2.12E+11	3.53E+10
1300	1.17E+10	7.24E+09	1.79E+09	3.40E+10	1.90E+09	2.83E+11	4.81E+10
1400	1.64E+10	1.01E+10	2.37E+09	4.95E+10	2.53E+09	3.71E+11	6.43E+10
1500	2.21E+10	1.38E+10	3.07E+09	6.96E+10	3.29E+09	4.76E+11	8.39E+10
1600	2.94E+10	1.70E+10	3.89E+09	9.55E+10	4.20E+09	6.00E+11	1.07E+11
1700	3.82E+10	2.07E+10	4.85E+09	1.27E+11	5.23E+09	7.52E+11	1.35E+11

1800	4.86E+10	2.48E+10	5.95E+09	1.67E+11	6.47E+09	9.24E+11	1.68E+11
1900	6.11E+10	2.94E+10	7.20E+09	2.16E+11	7.84E+09	1.12E+12	2.06E+11
2000	7.56E+10	3.47E+10	8.61E+09	2.74E+11	9.41E+09	1.36E+12	2.50E+11

Table S14 The site-specific rate constants per hydrogen atom of H-atom abstraction reactions from cyclopentanol and cyclopentane by HO₂ radical calculated using MS-T-TST/Eckart method.

T (K)	R1	R2a	R2b	R3a	R3b	R4	R _{cpt}
Forward reactions							
200	1.18E+00	4.20E-05	2.97E-06	3.20E-03	3.89E-05	7.11E-11	1.62E-04
250	5.51E+01	9.67E-03	1.20E-03	3.44E-01	8.84E-03	7.15E-07	3.78E-02
300	9.84E+02	5.06E-01	8.50E-02	1.02E+01	4.49E-01	3.93E-04	2.01E+00
350	9.52E+03	1.11E+01	2.17E+00	1.40E+02	9.13E+00	3.91E-02	4.26E+01
400	6.02E+04	1.33E+02	2.83E+01	1.17E+03	1.02E+02	1.34E+00	4.93E+02
450	2.81E+05	1.04E+03	2.28E+02	6.98E+03	7.33E+02	2.23E+01	3.72E+03
500	1.04E+06	5.86E+03	1.30E+03	3.22E+04	3.83E+03	2.22E+02	2.03E+04
550	3.20E+06	2.59E+04	5.66E+03	1.21E+05	1.56E+04	1.55E+03	8.62E+04
600	8.58E+06	9.44E+04	2.00E+04	3.88E+05	5.24E+04	7.89E+03	3.02E+05
650	2.04E+07	2.95E+05	6.04E+04	1.10E+06	1.51E+05	3.33E+04	8.99E+05
700	4.43E+07	8.05E+05	1.59E+05	2.73E+06	3.81E+05	1.12E+05	2.38E+06
750	8.90E+07	1.99E+06	3.75E+05	6.21E+06	8.72E+05	3.37E+05	5.66E+06
800	1.67E+08	4.47E+06	8.06E+05	1.31E+07	1.83E+06	9.03E+05	1.23E+07
850	2.96E+08	9.33E+06	1.61E+06	2.58E+07	3.56E+06	2.15E+06	2.49E+07
900	5.02E+08	1.83E+07	3.01E+06	4.79E+07	6.52E+06	4.75E+06	4.72E+07
950	8.10E+08	3.38E+07	5.33E+06	8.44E+07	1.13E+07	9.86E+06	8.47E+07
1000	1.27E+09	5.95E+07	8.94E+06	1.43E+08	1.87E+07	1.91E+07	1.45E+08
1100	2.81E+09	1.64E+08	2.25E+07	3.62E+08	4.56E+07	6.13E+07	3.78E+08
1200	5.62E+09	3.93E+08	4.93E+07	8.11E+08	9.81E+07	1.66E+08	8.64E+08
1300	1.04E+10	8.42E+08	9.80E+07	1.66E+09	1.90E+08	4.08E+08	1.78E+09
1400	1.79E+10	1.66E+09	1.78E+08	3.08E+09	3.41E+08	8.55E+08	3.37E+09

1500	2.91E+10	3.05E+09	3.02E+08	5.41E+09	5.72E+08	1.70E+09	5.96E+09
1600	4.52E+10	5.25E+09	4.84E+08	8.91E+09	9.06E+08	3.14E+09	9.91E+09
1700	6.74E+10	8.59E+09	7.41E+08	1.41E+10	1.37E+09	5.41E+09	1.57E+10
1800	9.74E+10	1.35E+10	1.09E+09	2.13E+10	1.99E+09	8.85E+09	2.39E+10
1900	1.36E+11	2.03E+10	1.54E+09	3.11E+10	2.80E+09	1.40E+10	3.52E+10
2000	1.85E+11	2.96E+10	2.12E+09	4.40E+10	3.83E+09	2.12E+10	5.01E+10

Reverse reactions

200	1.48E+06	6.95E+05	7.29E+05	9.96E+06	5.30E+05	7.50E+08	2.59E+06
250	4.26E+06	1.38E+06	1.54E+06	1.45E+07	1.16E+06	1.33E+09	6.35E+06
300	1.16E+07	2.92E+06	3.16E+06	2.35E+07	2.55E+06	2.31E+09	1.56E+07
350	2.86E+07	6.29E+06	6.26E+06	3.95E+07	5.37E+06	3.74E+09	3.57E+07
400	6.40E+07	1.29E+07	1.17E+07	6.69E+07	1.07E+07	5.82E+09	7.62E+07
450	1.32E+08	2.53E+07	2.06E+07	1.13E+08	1.98E+07	8.72E+09	1.52E+08
500	2.51E+08	4.64E+07	3.43E+07	1.89E+08	3.45E+07	1.26E+10	2.82E+08
550	4.46E+08	8.12E+07	5.40E+07	3.06E+08	5.68E+07	1.81E+10	4.90E+08
600	7.53E+08	1.36E+08	8.12E+07	4.82E+08	8.89E+07	2.46E+10	8.11E+08
650	1.21E+09	2.18E+08	1.18E+08	7.46E+08	1.33E+08	3.40E+10	1.27E+09
700	1.86E+09	3.35E+08	1.66E+08	1.10E+09	1.92E+08	4.38E+10	1.94E+09
750	2.78E+09	5.01E+08	2.27E+08	1.58E+09	2.69E+08	5.73E+10	2.84E+09
800	4.01E+09	7.24E+08	3.01E+08	2.23E+09	3.66E+08	7.39E+10	4.04E+09
850	5.63E+09	1.02E+09	3.92E+08	3.07E+09	4.85E+08	9.24E+10	5.61E+09
900	7.76E+09	1.41E+09	5.01E+08	4.14E+09	6.31E+08	1.15E+11	7.59E+09
950	1.04E+10	1.91E+09	6.30E+08	5.47E+09	8.04E+08	1.43E+11	1.01E+10
1000	1.38E+10	2.53E+09	7.75E+08	7.15E+09	1.01E+09	1.74E+11	1.31E+10
1100	2.28E+10	4.27E+09	1.14E+09	1.15E+10	1.52E+09	2.51E+11	2.13E+10
1200	3.57E+10	6.78E+09	1.60E+09	1.77E+10	2.18E+09	3.49E+11	3.27E+10
1300	5.36E+10	1.02E+10	2.17E+09	2.64E+10	3.00E+09	4.87E+11	4.81E+10
1400	7.73E+10	1.50E+10	2.85E+09	3.72E+10	4.01E+09	6.28E+11	6.81E+10
1500	1.08E+11	2.12E+10	3.64E+09	5.14E+10	5.21E+09	8.20E+11	9.37E+10

1600	1.46E+11	2.91E+10	4.55E+09	6.86E+10	6.60E+09	1.05E+12	1.25E+11
1700	1.94E+11	3.89E+10	5.59E+09	9.03E+10	8.19E+09	1.30E+12	1.63E+11
1800	2.52E+11	5.12E+10	6.77E+09	1.16E+11	9.98E+09	1.60E+12	2.09E+11
1900	3.20E+11	6.56E+10	8.04E+09	1.46E+11	1.20E+10	1.95E+12	2.63E+11
2000	4.00E+11	8.29E+10	9.46E+09	1.81E+11	1.42E+10	2.34E+12	3.26E+11

Table S15 The site-specific rate constants per hydrogen atom of H-atom abstraction reactions from cyclopentanol and cyclopentane by HO₂ radical calculated using SS-QH-TST method.

T (K)	R1	R2a	R2b	R3a	R3b	R4	<i>R_{cpt}</i>
Forward reactions							
200	2.22E-02	2.23E-07	1.16E-09	1.47E-04	1.03E-08	1.52E-11	5.48E-08
250	4.30E+00	2.66E-04	4.56E-06	4.71E-02	2.52E-05	2.32E-07	1.38E-04
300	1.58E+02	3.23E-02	1.20E-03	2.37E+00	4.82E-03	1.54E-04	2.82E-02
350	2.22E+03	1.06E+00	6.81E-02	4.14E+01	2.17E-01	1.69E-02	1.36E+00
400	1.70E+04	1.54E+01	1.47E+00	3.74E+02	3.94E+00	6.08E-01	2.64E+01
450	8.68E+04	1.29E+02	1.66E+01	2.17E+03	3.89E+01	1.03E+01	2.79E+02
500	3.32E+05	7.32E+02	1.19E+02	9.15E+03	2.50E+02	1.03E+02	1.93E+03
550	1.03E+06	3.14E+03	6.12E+02	3.08E+04	1.18E+03	6.98E+02	9.68E+03
600	2.73E+06	1.09E+04	2.44E+03	8.69E+04	4.39E+03	3.55E+03	3.83E+04
650	6.36E+06	3.19E+04	8.07E+03	2.14E+05	1.36E+04	1.43E+04	1.25E+05
700	1.34E+07	8.19E+04	2.28E+04	4.74E+05	3.64E+04	4.85E+04	3.56E+05
750	2.60E+07	1.89E+05	5.68E+04	9.62E+05	8.67E+04	1.41E+05	8.95E+05
800	4.71E+07	3.99E+05	1.28E+05	1.82E+06	1.88E+05	3.68E+05	2.03E+06
850	8.08E+07	7.81E+05	2.65E+05	3.21E+06	3.74E+05	8.67E+05	4.27E+06
900	1.32E+08	1.44E+06	5.10E+05	5.42E+06	6.98E+05	1.88E+06	8.36E+06
950	2.07E+08	2.52E+06	9.26E+05	8.74E+06	1.23E+06	3.80E+06	1.54E+07
1000	3.14E+08	4.19E+06	1.59E+06	1.36E+07	2.06E+06	7.22E+06	2.70E+07
1100	6.59E+08	1.04E+07	4.15E+06	2.97E+07	5.13E+06	2.25E+07	7.30E+07
1200	1.25E+09	2.29E+07	9.39E+06	5.89E+07	1.12E+07	5.97E+07	1.72E+08

1300	2.22E+09	4.54E+07	1.91E+07	1.07E+08	2.20E+07	1.40E+08	3.64E+08
1400	3.67E+09	8.36E+07	3.55E+07	1.83E+08	4.00E+07	2.94E+08	7.06E+08
1500	5.80E+09	1.44E+08	6.18E+07	2.96E+08	6.78E+07	5.73E+08	1.28E+09
1600	8.77E+09	2.36E+08	1.01E+08	4.56E+08	1.09E+08	1.04E+09	2.17E+09
1700	1.28E+10	3.68E+08	1.58E+08	6.78E+08	1.66E+08	1.79E+09	3.50E+09
1800	1.81E+10	5.54E+08	2.36E+08	9.75E+08	2.44E+08	2.92E+09	5.44E+09
1900	2.48E+10	8.04E+08	3.40E+08	1.36E+09	3.48E+08	4.58E+09	8.15E+09
2000	3.34E+10	1.14E+09	4.76E+08	1.85E+09	4.82E+08	6.92E+09	1.18E+10

Reverse reactions

200	2.78E+04	3.69E+03	2.85E+02	4.57E+05	1.40E+02	1.60E+08	8.74E+02
250	3.32E+05	3.79E+04	5.84E+03	1.98E+06	3.30E+03	4.32E+08	2.32E+04
300	1.86E+06	1.86E+05	4.46E+04	5.46E+06	2.74E+04	9.03E+08	2.19E+05
350	6.67E+06	6.01E+05	1.96E+05	1.17E+07	1.28E+05	1.62E+09	1.14E+06
400	1.81E+07	1.50E+06	6.10E+05	2.14E+07	4.14E+05	2.64E+09	4.08E+06
450	4.07E+07	3.14E+06	1.50E+06	3.53E+07	1.05E+06	4.03E+09	1.14E+07
500	8.01E+07	5.80E+06	3.14E+06	5.37E+07	2.26E+06	5.85E+09	2.68E+07
550	1.43E+08	9.85E+06	5.84E+06	7.78E+07	4.29E+06	8.16E+09	5.51E+07
600	2.39E+08	1.57E+07	9.91E+06	1.08E+08	7.44E+06	1.11E+10	1.03E+08
650	3.76E+08	2.36E+07	1.58E+07	1.45E+08	1.20E+07	1.46E+10	1.77E+08
700	5.63E+08	3.41E+07	2.38E+07	1.90E+08	1.83E+07	1.90E+10	2.90E+08
750	8.11E+08	4.76E+07	3.43E+07	2.45E+08	2.67E+07	2.40E+10	4.50E+08
800	1.13E+09	6.46E+07	4.78E+07	3.09E+08	3.76E+07	3.01E+10	6.67E+08
850	1.54E+09	8.56E+07	6.45E+07	3.82E+08	5.10E+07	3.73E+10	9.62E+08
900	2.04E+09	1.11E+08	8.48E+07	4.68E+08	6.76E+07	4.55E+10	1.34E+09
950	2.66E+09	1.42E+08	1.09E+08	5.67E+08	8.75E+07	5.50E+10	1.83E+09
1000	3.40E+09	1.78E+08	1.38E+08	6.80E+08	1.11E+08	6.58E+10	2.44E+09
1100	5.34E+09	2.71E+08	2.11E+08	9.47E+08	1.71E+08	9.21E+10	4.11E+09
1200	7.93E+09	3.95E+08	3.04E+08	1.29E+09	2.49E+08	1.25E+11	6.51E+09
1300	1.15E+10	5.53E+08	4.23E+08	1.70E+09	3.48E+08	1.67E+11	9.83E+09

1400	1.58E+10	7.54E+08	5.68E+08	2.21E+09	4.71E+08	2.16E+11	1.43E+10
1500	2.15E+10	1.00E+09	7.44E+08	2.81E+09	6.18E+08	2.76E+11	2.01E+10
1600	2.84E+10	1.31E+09	9.49E+08	3.51E+09	7.94E+08	3.47E+11	2.74E+10
1700	3.68E+10	1.67E+09	1.19E+09	4.34E+09	9.93E+08	4.31E+11	3.63E+10
1800	4.68E+10	2.10E+09	1.47E+09	5.30E+09	1.22E+09	5.27E+11	4.75E+10
1900	5.83E+10	2.60E+09	1.77E+09	6.38E+09	1.49E+09	6.38E+11	6.09E+10
2000	7.22E+10	3.19E+09	2.12E+09	7.60E+09	1.79E+09	7.63E+11	7.67E+10

11. Fitting parameters of modified Arrhenius equations

Table S16 Fitting parameters of modified Arrhenius equations of the MS-T-CVT/SCT rate constants per H-atom at 200–2000 K^a.

	Forward reactions			Reverse reactions		
	A	n	E	A	n	E
R1	1.37×10^{-4}	4.662	7.468	2.32×10^{-3}	4.206	2.032
R2a	1.49×10^{-8}	5.811	8.994	7.96×10^{-7}	5.108	-0.284
R2b	8.28×10^{-4}	4.15	11.565	5.07×10^{-2}	3.457	1.293
R3a	1.76×10^{-10}	6.429	6.594	1.80×10^{-8}	5.721	-1.767
R3b	1.01×10^{-4}	4.469	10.312	8.02×10^{-3}	3.758	1.254
R4	5.01×10^{-3}	4.375	16.466	3.23×10^{-2}	4.182	-0.607
<i>Rcpt</i>	3.17×10^{-4}	4.597	10.396	4.94×10^{-2}	3.877	1.523

^a Rate constants are in the unit of $\text{cm}^3 \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$. E is in the unit of $\text{kcal} \cdot \text{mol}^{-1}$.

12. Temperature-dependent activation energies

From Fig. 17, significant discrepancies of computed activation energies are observed between MS-T-CVT/SCT and SS-QH-TST results. For example, R3a and Rcpt show the largest discrepancies of above two methods with a difference range of -3.78 – 5.55 and -5.22 – -1.68 kcal/mol respectively at 200 – 2000 K. The quantum mechanical tunneling effect is mainly responsible for those deviations at low temperatures, while the deviations noted at high temperatures should be mainly attributed to the importance of anharmonicity effect. The numerical values of activation energies in tabular form are provided in Tables S17. From Fig. S4, it can be noted that activation energies derived from MS-LH-CVT/SCT generally deviates from those obtained by more accurate MS-T-CVT/SCT above 400 K with the maximum deviation being less than 2.02 kcal/mol due to the torsional anharmonicity.

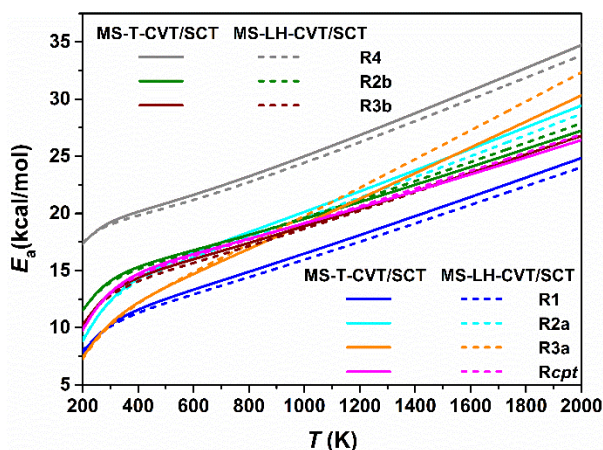


Fig. S4 The activation energies for the forward site-specific reactions for the H-atom abstraction from cyclopentanol and cyclopentane by HO_2 radical derived from MS-T-CVT/SCT and MS-LH-CVT/SCT rate constants.

Table S17 The temperature-dependent activation energies for H-atom abstraction reactions from cyclopentanol and cyclopentane by HO_2 radical calculated using MS-T-CVT/SCT method.

T (K)	R1	R2a	R2b	R3a	R3b	R4	Rcpt
Forward reactions							
200	7.83	8.83	11.51	7.39	10.22	17.33	9.79

250	9.29	10.95	13.13	9.13	11.94	18.55	11.82
300	10.28	12.43	14.14	10.41	13.04	19.25	13.15
350	11.01	13.50	14.81	11.40	13.80	19.74	14.06
400	11.58	14.32	15.31	12.20	14.37	20.14	14.73
450	12.07	14.98	15.73	12.90	14.84	20.51	15.25
500	12.51	15.56	16.10	13.53	15.25	20.88	15.69
550	12.93	16.07	16.44	14.13	15.63	21.24	16.08
600	13.33	16.56	16.78	14.70	15.99	21.62	16.44
650	13.72	17.02	17.11	15.26	16.35	22.01	16.78
700	14.11	17.47	17.44	15.81	16.71	22.41	17.11
750	14.50	17.91	17.78	16.35	17.06	22.82	17.45
800	14.90	18.36	18.12	16.90	17.42	23.24	17.78
850	15.29	18.80	18.46	17.44	17.78	23.67	18.11
900	15.68	19.24	18.81	17.98	18.14	24.10	18.44
950	16.08	19.68	19.16	18.53	18.51	24.54	18.78
1000	16.48	20.13	19.52	19.08	18.88	24.99	19.12
1100	17.29	21.02	20.25	20.17	19.63	25.91	19.81
1200	18.10	21.93	20.99	21.28	20.39	26.85	20.51
1300	18.93	22.84	21.74	22.39	21.17	27.80	21.22
1400	19.76	23.77	22.51	23.51	21.95	28.76	21.94
1500	20.59	24.70	23.28	24.64	22.74	29.74	22.67
1600	21.44	25.63	24.06	25.77	23.54	30.72	23.41
1700	22.28	26.58	24.85	26.90	24.35	31.71	24.16
1800	23.13	27.53	25.64	28.04	25.16	32.71	24.91
1900	23.99	28.48	26.44	29.18	25.97	33.72	25.66
2000	24.84	29.44	27.24	30.32	26.79	34.72	26.42
Reverse reactions							
200	2.74	0.78	1.83	0.33	1.78	0.86	1.70
250	3.71	1.50	2.62	0.75	2.63	1.32	2.68

300	4.49	2.34	3.28	1.31	3.38	1.81	3.59
350	5.13	3.20	3.83	1.98	4.01	2.31	4.38
400	5.67	4.03	4.30	2.72	4.55	2.78	5.04
450	6.13	4.80	4.71	3.48	5.01	3.24	5.59
500	6.56	5.49	5.07	4.24	5.42	3.69	6.05
550	6.96	6.12	5.41	4.98	5.79	4.11	6.46
600	7.34	6.68	5.72	5.67	6.13	4.53	6.82
650	7.71	7.19	6.02	6.33	6.46	4.93	7.14
700	8.07	7.65	6.32	6.94	6.77	5.33	7.44
750	8.43	8.07	6.60	7.51	7.08	5.73	7.72
800	8.79	8.45	6.89	8.04	7.38	6.12	7.99
850	9.14	8.82	7.17	8.53	7.67	6.50	8.25
900	9.50	9.16	7.45	8.99	7.96	6.89	8.50
950	9.85	9.48	7.73	9.43	8.25	7.27	8.74
1000	10.21	9.79	8.01	9.84	8.54	7.66	8.99
1100	10.93	10.38	8.57	10.60	9.12	8.42	9.46
1200	11.64	10.95	9.13	11.29	9.70	9.19	9.94
1300	12.37	11.49	9.69	11.94	10.28	9.96	10.41
1400	13.09	12.02	10.26	12.56	10.86	10.73	10.88
1500	13.83	12.55	10.82	13.15	11.45	11.50	11.36
1600	14.56	13.07	11.39	13.73	12.03	12.27	11.83
1700	15.30	13.59	11.97	14.29	12.62	13.05	12.31
1800	16.03	14.11	12.54	14.85	13.22	13.83	12.79
1900	16.78	14.63	13.12	15.39	13.81	14.60	13.28
2000	17.52	15.15	13.70	15.94	14.41	15.38	13.76

13. Optimized geometries and calculated non-scaled frequencies

Table S18 Geometries and non-scaled frequencies of the lowest energy conformers for reaction species obtained at the level of M06-2X/MG3S.

Species	Geometries (Å)			Frequencies (cm ⁻¹)			
CPL	C	-0.782613	0.012112	0.352609	35.6956	196.4621	256.0791
	C	0.021455	-1.208032	-0.083608	364.3953	475.7271	544.9814
	C	1.496035	-0.751886	-0.049835	618.1056	771.5156	824.7866
	C	1.456975	0.790531	0.107336	897.2032	909.6508	963.1951
	C	0.015417	1.177313	-0.226711	976.6219	992.9944	1059.5563
	H	-0.776584	0.084525	1.448211	1091.9917	1142.5808	1195.4343
	H	-0.290743	-1.451078	-1.100448	1208.0317	1213.2279	1269.9522
	H	-0.177580	-2.078903	0.537472	1278.5612	1304.4364	1322.5456
	H	2.041814	-1.212185	0.771814	1334.5753	1344.6950	1385.5778
	H	2.007947	-1.038837	-0.966583	1433.1669	1489.8754	1499.2542
	H	1.678993	1.065762	1.139405	1503.2275	1527.5451	3001.0766
	H	2.186796	1.295782	-0.521905	3092.8853	3113.8859	3118.7123
	H	-0.278873	2.147130	0.175805	3131.9035	3142.9099	3901.8707
	H	-0.145353	1.191000	-1.307640			
	O	-2.109772	-0.098609	-0.118277			
H	-2.611858	0.665443	0.171337				
CPT	C	0.618087	-1.118651	0.154629	10.6552	278.7406	548.0241
	C	1.270328	0.274443	-0.010139	614.9242	770.8019	829.0240
	C	0.097605	1.278780	-0.134710	880.2642	902.9477	917.7995
	C	-1.154498	0.482971	0.253634	926.1354	971.9984	1004.2297
	C	-0.842718	-0.921079	-0.263176	1048.7612	1066.9394	1186.4214
	H	1.125055	-1.890525	-0.422018	1208.9301	1232.4704	1241.3938
	H	0.651758	-1.423735	1.201796	1288.5041	1309.3598	1328.2135
	H	1.903268	0.309592	-0.895651	1345.1007	1353.0713	1355.0768
	H	1.907863	0.509196	0.840773	1490.4000	1495.9406	1501.9301

	H	0.239584	2.166840	0.478767	1502.8725	1529.0979	3053.9669
	H	0.003623	1.614489	-1.168399	3061.1359	3071.0176	3072.5033
	H	-1.259184	0.453582	1.341080	3088.0105	3110.0535	3119.3282
	H	-2.070949	0.905438	-0.156164	3122.4703	3124.3765	3137.4407
	H	-1.507162	-1.688721	0.131294			
	H	-0.926682	-0.934928	-1.352902			
	O	0.054956	-0.598793	0.000000	1264.6120	1470.4057	3705.3984
HO ₂	H	-0.879301	-0.866630	0.000000			
	O	0.054956	0.707122	0.000000			
	C	0.035985	0.484096	0.118902	-1526.9303	48.0090	59.2146
	C	1.127199	0.901151	-0.858492	113.2927	154.0734	223.9209
	C	2.322711	-0.016400	-0.525983	263.1832	343.9754	385.8361
	C	1.726007	-1.159693	0.310591	416.5299	522.0504	549.6377
	C	0.654440	-0.456211	1.141345	557.4677	633.9652	784.2717
	H	-0.771201	-0.267806	-0.490387	847.7925	882.5865	913.7028
	H	1.354310	1.957834	-0.715164	947.8097	972.9861	1027.1018
	H	0.793666	0.780938	-1.889177	1047.8605	1097.3565	1109.0104
	H	2.841933	-0.370120	-1.414054	1166.6131	1193.1806	1221.2464
SP1	H	3.046694	0.530082	0.079674	1237.2373	1250.2592	1280.3740
	H	1.252332	-1.897239	-0.340784	1301.9414	1330.0370	1343.1065
	H	2.468744	-1.676741	0.914539	1360.2311	1390.1065	1424.1692
	H	-0.078391	-1.127870	1.588626	1481.3191	1484.1154	1499.1072
	H	1.111889	0.143107	1.935663	1515.7364	1550.7096	3040.2686
	O	-0.727501	1.533804	0.579888	3069.7564	3077.8549	3081.6341
	H	-1.421839	1.178379	1.146533	3115.6572	3116.2062	3132.9252
	O	-2.772410	-0.362670	0.037842	3139.8828	3811.4081	3836.9425
	H	-3.188999	0.305717	-0.520471			
	O	-1.825988	-0.930377	-0.794378			
SP2a	C	-0.752149	1.001220	0.511378	-1931.7750	77.7307	141.4664

	C	-1.893862	0.437557	-0.330371	165.3507	181.7858	233.3039
	C	-1.354776	-0.910228	-0.816904	305.4973	399.9330	417.4988
	C	-0.632145	-1.471725	0.417606	450.4250	529.9998	583.4156
	C	-0.149935	-0.242327	1.171651	609.9429	760.6209	813.0708
	H	-1.092274	1.733398	1.246244	849.3582	863.7723	917.4198
	H	-2.170325	1.125259	-1.127547	934.9271	951.9190	1009.5983
	H	-2.763405	0.281249	0.311217	1032.0179	1050.5242	1077.7876
	H	-2.135919	-1.572981	-1.183555	1085.1934	1161.0518	1185.8051
	H	-0.643094	-0.754722	-1.627578	1198.2865	1238.8068	1262.6383
	H	-1.326476	-2.035724	1.046380	1294.1339	1312.9046	1341.8490
	H	0.185315	-2.144660	0.155521	1353.4317	1362.6840	1414.1814
	H	-0.174065	-0.280883	2.257671	1465.6883	1478.3655	1484.7179
	H	1.155598	-0.174363	0.930806	1487.8178	1508.4841	3050.9282
	O	0.156248	1.636885	-0.393062	3065.1522	3078.1153	3091.1561
	H	0.933193	1.911962	0.103876	3103.8683	3135.3448	3142.7245
	O	2.018646	-0.489204	-0.861011	3145.0287	3728.0988	3857.7727
	H	1.553647	0.258186	-1.270408			
	O	2.221982	-0.051893	0.433724			
	C	1.194862	0.580044	-0.332209	-1839.5722	39.3285	59.3994
	C	1.392301	-0.876566	-0.780724	106.8795	126.3838	222.3939
	C	0.166043	-1.634507	-0.264439	289.3520	294.4530	389.2952
	C	-0.117645	-0.953353	1.077975	409.4678	460.6392	554.0792
	C	0.130309	0.500218	0.761161	600.4374	640.3489	808.0425
SP2b	H	0.848849	1.201293	-1.163872	865.0359	877.0887	924.6861
	H	2.293339	-1.238981	-0.282390	932.8102	947.4869	1033.4557
	H	1.542629	-0.965344	-1.854221	1047.7214	1073.9077	1085.4118
	H	-0.687649	-1.483723	-0.927530	1092.8918	1163.4558	1190.1427
	H	0.339546	-2.705010	-0.174851	1211.4717	1236.1700	1271.3284
	H	-1.118972	-1.147854	1.462438	1282.7727	1312.2247	1334.6812

	H	0.599289	-1.289496	1.836035	1347.3230	1367.1235	1418.9632
	H	-0.966770	0.869826	0.145103	1422.3635	1457.9418	1467.7190
	H	0.221950	1.212847	1.578021	1494.3004	1511.1321	3025.9680
	O	2.435184	1.077205	0.149187	3037.7388	3077.3154	3081.7875
	H	2.370566	2.026643	0.269872	3107.6305	3134.9392	3137.9393
	O	-2.801785	0.022346	-0.180523	3144.3723	3817.8417	3900.6895
	H	-3.367704	0.378958	0.514824			
	O	-1.967185	1.081177	-0.490416			
	C	1.258975	-0.853144	0.173172	-1905.5327	75.6924	136.3201
	C	1.508852	0.048920	-1.030104	161.5966	201.8011	226.7204
	C	0.561139	1.253308	-0.837022	322.8239	360.1889	390.8355
	C	0.191767	1.234706	0.636363	430.7753	555.3893	632.8350
	C	0.993144	0.137525	1.307179	676.0701	740.8140	796.5126
	H	2.100946	-1.516424	0.381015	838.1422	877.3951	913.6891
	H	1.344853	-0.487814	-1.962519	924.6376	968.1293	1003.5876
	H	2.548460	0.377164	-1.009516	1036.7658	1060.0461	1083.7726
	H	1.035313	2.193332	-1.121222	1095.2383	1151.9557	1194.3138
SP3a	H	-0.334190	1.157086	-1.456166	1220.4055	1229.8977	1252.0691
	H	0.100293	2.184828	1.154181	1278.5145	1312.6802	1328.3302
	H	-1.062803	0.777261	0.669704	1356.5944	1380.9181	1418.5193
	H	1.950000	0.525596	1.672392	1470.1210	1472.2677	1488.4342
	H	0.483561	-0.318128	2.158962	1494.8715	1503.9107	3036.6022
	O	0.102694	-1.640518	-0.115157	3059.3663	3071.1518	3087.4710
	H	-0.242105	-2.002169	0.705960	3090.0880	3099.5264	3141.6604
	O	-2.200449	-0.155362	-0.727030	3153.9324	3689.7569	3876.1353
	H	-1.570325	-0.890938	-0.813731			
	O	-2.081903	0.179919	0.607614			
SP3b	C	-1.005608	-0.598095	-0.220620	-1833.6048	60.8773	67.7310
	C	-1.560792	0.757290	-0.645958	105.1100	153.0701	199.4323

	C	-0.492746	1.774954	-0.204208	283.3724	295.2563	366.9966
	C	0.346855	1.033905	0.834737	419.6732	471.4151	555.6924
	C	-0.324160	-0.287476	1.114708	578.0827	650.5826	776.3483
	H	-0.243807	-0.928472	-0.935639	832.4807	895.8679	911.1770
	H	-2.492299	0.912630	-0.098227	956.1129	981.4739	992.2447
	H	-1.786636	0.799634	-1.708830	1067.2205	1088.0043	1093.2030
	H	0.127179	2.093506	-1.044465	1142.9051	1163.6663	1184.1979
	H	-0.935785	2.678721	0.215185	1222.6673	1237.7229	1273.4981
	H	1.416992	0.688362	0.181030	1277.9880	1305.2852	1327.8565
	H	0.741836	1.601291	1.673091	1340.4635	1380.7095	1422.0659
	H	0.364275	-1.067342	1.442500	1442.8654	1454.9165	1470.1871
	H	-1.099627	-0.172776	1.881526	1483.9233	1510.3305	3023.9280
	O	-2.053878	-1.539535	-0.140101	3040.9295	3065.9046	3077.0543
	H	-1.682747	-2.413755	-0.007848	3100.7359	3105.8256	3144.0647
	O	2.344798	-1.100378	-0.240046	3145.1933	3817.8785	3907.0093
	H	3.061048	-1.169947	0.402680			
	O	2.302614	0.251748	-0.528973			
SP4	C	0.162782	0.431917	0.169129	-1820.3992	20.6058	57.0103
	C	0.472609	-0.800219	-0.678690	74.8366	104.4273	181.8170
	C	1.793077	-1.290477	-0.081883	246.6031	344.1028	433.9478
	C	2.558565	-0.002561	0.311635	464.5939	536.4825	613.9651
	C	1.541448	1.154065	0.219070	668.3122	768.6106	817.5748
	H	-0.100999	0.132654	1.194260	844.8414	878.2522	903.0793
	H	0.600151	-0.474866	-1.713530	959.0442	970.3815	993.4843
	H	-0.331238	-1.533634	-0.643265	1051.2680	1061.3521	1114.7558
	H	1.593244	-1.891251	0.805731	1161.5567	1192.4709	1203.6744
	H	2.354643	-1.917305	-0.771297	1217.5872	1260.9803	1287.2419
	H	2.966361	-0.083169	1.317578	1295.3095	1310.8920	1329.7190
	H	3.396429	0.184039	-0.357774	1342.3500	1394.0565	1434.8776

	H	1.592596	1.860295	1.043548	1488.3607	1495.8240	1502.0372
	H	1.650334	1.707165	-0.713078	1507.4741	1524.4635	2979.7957
	O	-0.762323	1.300160	-0.343854	3071.4371	3082.0634	3089.7792
	H	-1.848100	0.702453	-0.471292	3097.3117	3122.2284	3135.6835
	O	-2.542369	-0.723020	0.712554	3141.3222	3157.7557	3806.3757
	H	-3.053174	-0.217495	1.357896			
	O	-2.694201	-0.005294	-0.454242			
SPcpt	C	1.026245	1.298892	-0.055285	-1818.0308	32.7307	53.0157
	C	0.247519	0.577258	1.024823	120.6215	173.9703	261.7063
	C	0.620720	-0.895677	0.971910	319.8466	408.1705	535.6541
	C	1.505466	-1.039243	-0.285885	582.9517	649.9417	784.8498
	C	1.202633	0.211881	-1.118376	839.1089	875.7392	912.6356
	H	0.519754	2.192165	-0.419463	918.8596	930.5911	960.6089
	H	2.002578	1.607671	0.336194	1013.7525	1048.9626	1068.6914
	H	-0.970872	0.632277	0.571588	1090.0679	1165.9206	1199.6829
	H	0.161862	1.048109	2.000931	1207.6041	1233.1599	1244.6434
	H	1.134727	-1.211582	1.881109	1292.8514	1302.9300	1337.1531
	H	-0.273029	-1.518976	0.887395	1353.1848	1354.6322	1417.5266
	H	2.557881	-1.036436	0.003761	1453.7404	1476.7349	1477.4259
	H	1.315272	-1.964207	-0.826460	1495.6385	1511.7360	3024.1649
	H	1.982232	0.440214	-1.842896	3055.0241	3068.1437	3077.3289
	H	0.261703	0.082210	-1.656412	3090.3878	3114.1870	3129.6020
	O	-2.153586	-0.641497	-0.532667	3136.7789	3143.3810	3818.0776
	H	-2.713300	-1.103299	0.103331			
	O	-2.045701	0.630646	-0.000108			
Prdl	C	0.795099	0.003992	-0.228268	99.8796	241.3570	304.6180
	C	-0.031846	-1.241841	-0.151186	315.1142	386.4236	555.5979
	C	-1.420149	-0.719061	0.265898	566.4025	780.2841	849.7756
	C	-1.435246	0.747993	-0.190163	871.3560	910.1371	922.1606

	C	-0.006804	1.223582	0.101564	969.0797	1025.2574	1042.8062
	H	0.386389	-1.951378	0.567072	1107.7178	1138.3364	1168.2400
	H	-0.073249	-1.757950	-1.115327	1226.3258	1247.2071	1283.3246
	H	-2.241077	-1.300718	-0.149252	1299.2694	1323.1664	1343.0390
	H	-1.507846	-0.754216	1.353256	1387.7901	1420.9493	1484.6864
	H	-1.623387	0.802667	-1.263754	1486.9682	1495.7325	1515.7310
	H	-2.194905	1.341826	0.314651	2967.3266	3030.3558	3062.7146
	H	0.278758	2.106235	-0.475714	3063.9954	3076.7379	3079.3175
	H	0.099291	1.482107	1.166401	3125.8674	3133.6570	3896.6340
	O	2.117547	-0.102567	0.093955			
	H	2.529324	0.763968	0.063958			
	C	-0.875406	0.095600	0.496993	129.4074	201.7778	215.4982
	C	0.022934	-1.140370	0.517363	310.3262	415.8217	461.6257
	C	1.159192	-0.778300	-0.446573	597.9539	768.8243	835.4217
	C	1.426206	0.708855	-0.149951	851.1764	914.5582	917.4343
	C	0.098494	1.214105	0.313508	934.9300	988.4511	1041.5551
	H	-1.478107	0.194285	1.403988	1045.9214	1053.6575	1149.7748
	H	-0.527759	-2.034473	0.231570	1190.3160	1233.0802	1246.0240
Prd2a	H	0.414972	-1.279734	1.526904	1308.8460	1311.9870	1345.2175
	H	2.041715	-1.401699	-0.318439	1349.0741	1376.5713	1403.5946
	H	0.809880	-0.890224	-1.472669	1473.0914	1485.2191	1505.3320
	H	2.175387	0.814499	0.645351	3001.8660	3048.0225	3074.0800
	H	1.817823	1.254127	-1.010997	3076.0585	3093.1708	3135.6965
	H	-0.127722	2.251175	0.514989	3143.3476	3216.7891	3893.4351
	O	-1.752192	-0.041501	-0.631250			
	H	-2.097181	0.824716	-0.858734			
	C	-0.821964	-0.029013	0.401859	99.7753	230.3090	260.2615
Prd2b	C	0.059714	-1.177807	-0.097016	326.5283	389.9748	512.7127
	C	1.491404	-0.678712	0.110593	564.5360	637.0350	844.6876

	C	1.407892	0.815402	-0.251701	878.0415	898.9953	927.0768
	C	0.026291	1.182513	0.172116	955.4940	1015.1617	1042.2392
	H	-1.040462	-0.156234	1.472150	1070.2151	1089.6337	1127.7755
	H	-0.147390	-1.298722	-1.162359	1207.7605	1229.8608	1267.5705
	H	-0.155310	-2.121474	0.399758	1301.1248	1307.3641	1326.9322
	H	1.774736	-0.782927	1.159667	1349.5958	1364.8003	1417.6764
	H	2.220863	-1.223501	-0.485642	1474.9129	1494.8475	1508.9793
	H	2.183108	1.418717	0.223837	2971.0212	2994.0325	3067.6195
	H	1.533356	0.947549	-1.334697	3077.5234	3084.2996	3129.6700
	H	-0.346109	2.192882	0.259476	3141.2266	3219.3313	3902.3228
	O	-2.049172	-0.039789	-0.319118			
	H	-2.609429	0.667731	0.005642			
	C	-0.859657	-0.020538	0.473328	155.1009	186.6677	291.9018
	C	0.186884	-1.124889	0.575770	311.9239	394.2170	416.3387
	C	1.298693	-0.667076	-0.383905	657.3364	766.3033	826.6582
	C	1.224929	0.823537	-0.303096	864.2753	910.9330	931.2909
	C	-0.021647	1.265374	0.393667	940.4613	980.3252	1038.4237
	H	-1.550512	-0.018728	1.320485	1048.8043	1061.0413	1122.4927
	H	-0.237836	-2.094949	0.325981	1178.0583	1226.3688	1250.2870
Prd3a	H	0.566356	-1.163104	1.598047	1282.8912	1314.0478	1326.5760
	H	2.278834	-1.065151	-0.114245	1361.0867	1389.2258	1417.5730
	H	1.084858	-1.016105	-1.400511	1465.5445	1473.4677	1491.2811
	H	1.943734	1.494469	-0.746235	2998.7122	3020.2720	3053.4029
	H	0.184743	1.638145	1.405546	3055.5395	3074.2495	3088.1740
	H	-0.556605	2.066252	-0.125566	3143.5276	3233.6956	3901.9776
	O	-1.569342	-0.250306	-0.735098			
	H	-2.134051	0.503166	-0.917299			
Prd3b	C	-0.747121	-0.034145	0.356902	161.1542	180.3599	270.9586
	C	0.129850	-1.164994	-0.168051	312.4708	368.2491	475.1089

	C	1.560114	-0.658698	0.068121	554.1091	660.2944	822.0205
	C	1.422927	0.829002	-0.041938	885.5880	909.2832	932.0226
	C	-0.011301	1.235656	-0.100489	968.1214	1003.4081	1052.5547
	H	-0.755708	-0.066009	1.453482	1069.8012	1105.3188	1135.9392
	H	-0.067171	-1.265685	-1.237424	1185.4367	1231.7855	1273.3346
	H	-0.087127	-2.118428	0.308844	1276.3644	1308.1819	1328.8415
	H	1.913805	-0.950054	1.065217	1348.7786	1384.7416	1434.2650
	H	2.277049	-1.077307	-0.641160	1474.5205	1481.2498	1506.7505
	H	2.254705	1.514874	-0.074244	2987.4296	3002.2378	3013.2817
	H	-0.245534	2.111885	0.508953	3068.4101	3070.3108	3081.0784
	H	-0.332782	1.463465	-1.126447	3140.6223	3232.7175	3902.6688
	O	-2.059034	-0.172152	-0.145037			
	H	-2.611782	0.523541	0.215815			
	C	0.950227	0.019644	0.439271	60.4637	245.8863	362.2104
	C	0.005704	1.259512	0.202077	401.7924	561.3445	659.2387
	C	-1.390540	0.670508	-0.065719	802.0518	827.5951	852.4513
	C	-1.131543	-0.786914	-0.452997	889.8464	924.6615	937.7440
	C	-0.000079	-1.183919	0.490253	991.8479	1011.3524	1051.0647
	H	1.543808	0.154029	1.349495	1064.5585	1154.0131	1193.1303
	H	0.377427	1.824228	-0.651645	1235.2322	1246.7152	1274.8758
Prd4	H	0.039703	1.914591	1.069347	1301.4930	1323.7814	1328.5680
	H	-1.984537	0.701761	0.849189	1349.3044	1386.5378	1483.0029
	H	-1.931493	1.227798	-0.828028	1484.4368	1494.6600	1515.7429
	H	-2.013573	-1.418272	-0.361873	3031.0267	3065.7814	3072.3634
	H	-0.778855	-0.842476	-1.483993	3081.6011	3096.0597	3126.0708
	H	-0.376485	-1.296329	1.510098	3129.4338	3136.5689	3148.6041
	H	0.513604	-2.102800	0.212163			
	O	1.750974	-0.004439	-0.667758			
Prd-cpt	C	0.618087	-1.118651	0.154629	171.8126	247.2005	321.2383

	C	1.270328	0.274443	-0.010139	561.5318	657.1119	829.0402
	C	0.097605	1.278780	-0.134710	863.9802	898.3117	914.2029
	C	-1.154498	0.482971	0.253634	929.1983	938.7157	1016.3723
	C	-0.842718	-0.921079	-0.263176	1043.3653	1051.6096	1097.2218
	H	1.125055	-1.890525	-0.422018	1190.7801	1229.6192	1245.2534
	H	0.651758	-1.423735	1.201796	1297.2938	1306.1922	1334.7216
	H	1.903268	0.309592	-0.895651	1353.3197	1373.5668	1477.7451
	H	1.907863	0.509196	0.840773	1479.9569	1494.4942	1510.6119
	H	0.239584	2.166840	0.478767	2990.8450	2991.6356	3060.8882
	H	0.003623	1.614489	-1.168399	3065.2933	3076.0623	3076.7877
	H	-1.259184	0.453582	1.341080	3124.0819	3130.1926	3230.6070
	H	-2.070949	0.905438	-0.156164			
	H	-1.507162	-1.688721	0.131294			
	H	-0.926682	-0.934928	-1.352902			
H ₂ O ₂	O	0.000000	-0.710054	-0.058025	381.0059	1046.6469	1368.5939
	H	-0.785844	-0.903139	0.464198	1478.6921	3855.0882	3855.8399
	O	0.000000	0.710054	-0.058025			
	H	0.785844	0.903139	0.464198			