Supplementary Material for

Theoretical investigation on degradation of $CH{\equiv}CCH_2OH$ by NO_3 radicals in the atmosphere

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Computational details of rate constants.

For SCHEME 1:

$$k_{\text{TS1-ir-r}}(T,P)=\frac{\alpha_a}{h}\frac{Q_t^{\neq}Q_r^{\neq}}{Q_{\text{CH}\equiv\text{CCH}_2\text{OH}}Q_{\text{NO}_3}}e^{-E_a/RT}\times\int_0^{\infty}\frac{\omega}{\text{X}_2}N_a(E^{\neq})e^{-E^{\neq}/RT}dE^{\neq} \quad (1)$$

$$k_{\text{TS1-IR-R-TS2-IR-R}}(T,P)=\frac{\alpha_a}{h}\frac{Q_t^{\neq}Q_r^{\neq}}{Q_{\text{CH}\equiv\text{CCH}_2\text{OH}}Q_{\text{NO}_3}}e^{-E_a/RT}\times\int_0^{\infty}\frac{\omega\text{X}_1}{\text{X}_2}N_a(E^{\neq})e^{-E^{\neq}/RT}dE^{\neq} \quad (2)$$

$$k_{\text{P1(CH}_2\text{CONO}_2\text{CHO+H)}}(T,P)=\frac{\alpha_a}{h}\frac{Q_t^{\neq}Q_r^{\neq}}{Q_{\text{CH}_2=\text{CH}=\text{CH}_2}Q_{\text{NO}_3}}e^{-E_a/RT}\times\int_0^{\infty}\frac{k_4(E)\text{X}_1}{\text{X}_2}N_a(E^{\neq})e^{-E^{\neq}/RT}dE^{\neq} \quad (3)$$

Where

$X_1 = k_2(E)/(k_3(E) + k_4(E) + \omega)$

$X_2 = k_1(E) + k_2(E) - k_3(E)*X_1 + \omega$

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For SCHEME 2:

$$k_{\text{TS2-IF-F}}(T,P)=\frac{\alpha_a}{h}\frac{Q_t^{\neq}Q_r^{\neq}}{Q_{\text{CH}\equiv\text{CCH}_2\text{OH}}Q_{\text{NO}_3}}e^{-E_a/RT}\times\int_0^{\infty}\frac{\omega}{k_1(E)+k_2(E)+\omega}N_a(E^{\neq})e^{-E^{\neq}/RT}dE^{\neq} \tag{4}$$

$$k_{\text{P(CHOCCH}_2\text{OH+NO}_2)}(T,P)=\frac{\alpha_a}{h}\frac{Q_t^{\neq}Q_r^{\neq}}{Q_{\text{CH}\equiv\text{CHCH}_2\text{OH}}Q_{\text{NO}_3}}e^{-E_a/RT}\times\int_0^{\infty}\frac{k_2(E)}{k_1(E)+k_2(E)+\omega}N_a(E^{\neq})e^{-E^{\neq}/RT}dE^{\neq} \tag{5}$$

The microcanonical rate constant is calculated using the RRKM theory as follows:

$$k_i(E)=\alpha_i C_i N_i(E_i^{\neq})/h\rho_j(E_j) \tag{6}$$

In the above equations, α_a is the statistical factor for the reaction path a, and α_i is the statistical factor (degeneracy) for the *i*th reaction path; E_a is the energy barrier for the reaction step a. Q_{NO_3} and $Q_{\text{CH}\equiv\text{CHCH}_2\text{OH}}$ are the total partition function of NO_3 and $CH{\equiv}CCH_2OH$, respectively; $Q_t^{\neq}$ and $Q_r^{\neq}$ are the translational and rotational partition functions of entrance transition state, respectively; $N_a(E^{\neq})$ is the number of state for the association transition state with excess energy $E^{\neq}$ above the association barrier. $k_i(E)$ is the energy-specific rate constant for the *i*th channel and C_i is the ratio of the overall rotational partition function of the TS_i and IM_j; $N_i(E_i^{\neq})$ is the number of states at the energy above the barrier height for transition state *i*; $\rho_j(E_j)$ is the density of states at energy E_j of the intermediate. The density of states and the number of states are calculated using the extended Beyer-Swinehart algorithm.

The rate coefficients for the direct hydrogen abstraction routes can be readily obtained using the conventional transition-state theory [1]:

$$k_{abs}(T) = \kappa_1 \frac{k_B T}{h} \frac{Q_{TS}^{\neq}}{Q_{CH\equiv CCH_2OH} Q_{NO_3}} e^{-E_1/(RT)} \quad (7)$$

where κ_1 is the tunneling factor, k_B and h are Boltzmann and Planck constants, respectively. $Q_{TS}^{\neq}$, $Q_{CH\equiv CCH_2OH}$ and Q_{NO_3} are the h-TS1 and h-TS3, $CH\equiv CCH_2OH$ and NO_3 partition functions, respectively. E_1 is the barrier of h-TS1 and h-TS3. The unsymmetrical Eckart potential model is employed to estimate κ_1 [2,3].

[1] I. W. M. Smith, Kinetics and Dynamics of Elementary Gas Reactions; Butterworth, London, 1980, p118.

[2] H. S. Johnston and J. Heicklen, Tunnelling Corrections for Unsymmetrical Eckart Potential Energy Barriers. J. Phys. Chem. 66 (1962)532–533.

[3] C. Eckart, The Penetration of a Potential Barrier by Electrons. Phys. Rev. 35(1930)1303–1309.

Gibbs free energy of solute in aqueous solution can be calculated as follows (Ribeiro et al., 2011):

$$G_{aq} = G_g + G_{diss}$$

$$G_{diss} = sp_{aq} - sp_g + 1.89 \text{ (kcal/mol)}$$

Where G_{aq} is Gibbs free energy of solute in aqueous solution, G_g is Gibbs free energy of solute in gas-phase, G_{diss} is dissolved free energy of solute, and sp_{aq} is single point energy of solute in aqueous solution calculated at M06-2X/6-311++G(3df,2p) level with "PCM" model based on the structure optimized in gas-phase at M06-2X/6-311G(d,p) level. And sp_g is single point energy of solute in gas-phase calculated at M06-2X/6-311G(d,p) level.

References

Ribeiro, R.F., Marenich, A.V., Cramer, C.J., Truhlar, D.G., 2011. Use of Solution-Phase Vibrational Frequencies in Continuum Models for the Free Energy of Solvation. J. Phys. Chem. B. 115, 14556-14562.

Table S1. The values of G_{aq}, G_g, sp_{aq} and sp_g for the reactants, intermediates, transition states and products. Units of these energies are hartree.

Species	G_g	sp_{aq}	sp_g	G_{aq}
CH≡CCH$_2$OH	-191.52	-191.49	-191.49	-191.52
NO$_3$	-279.86	-279.83	-279.83	-279.86
h-TS2-if-f	-471.32	0.073322	-471.28	0.035666
IM1	-471.38	-471.36	-471.35	-471.39
IM2	-471.38	-471.36	-471.34	-471.39
IM3	-471.40	-471.37	-471.36	-471.40
IM4	-471.43	-471.41	-471.40	-471.44
IM5	-471.40	-471.37	-471.36	-471.40
TS1	-471.35	-471.32	-471.32	-471.36
TS2	-471.34	—	-471.31	—
TS3	-471.34	-471.32	-471.31	-471.35
TS4	-471.32	—	-471.29	—
TS5	-471.36	-471.33	-471.32	-471.36
TS6	-471.33	-471.30	-471.30	-471.33
TS7	-471.36	-471.34	-471.33	-471.36
TS8	-471.42	-471.39	-471.38	-471.42
TS9	-471.36	-471.33	-471.32	-471.36
TS10	-471.36	-471.33	-471.32	-471.37
TS11	-471.32	-471.30	-471.29	-471.34
TS12	-471.33	-471.30	-471.29	-471.34
TS13	-471.36	-471.33	-471.33	-471.37
H-TS1	-471.35	-471.32	-471.32	-471.36
H-TS2	-471.32	-471.30	-471.28	-471.33
H-TS3	-471.34	-471.29	-471.31	-471.33
CHONO$_2$CHCHO	-470.87	-470.85	-470.84	-470.88
CH$_2$CONO$_2$CHO	-470.88	-470.85	-470.84	-470.88
CHOCHCHOH	-266.68	-266.67	-266.66	-266.70
CH$_2$COHCHO	-266.69	-266.67	-266.66	-266.70
CHCOCH$_2$OH	-266.56	-266.54	-266.53	-266.57
CHCCHOH	-190.88	-190.86	-190.85	-190.89
CCCH$_2$OH	-190.80	-190.78	-190.78	-190.81
CHCCH$_2$O	-190.85	-190.83	-190.821	-190.85
CH$_2$OH	-114.87	-114.85	-114.85	-114.87
HCCO	-151.68	-151.66	-151.66	-151.68
HNO$_3$	-280.52	-280.50	-280.49	-280.52
NO$_2$	-204.81	-204.79	-204.79	-204.82
H	-0.51	-0.50	-0.50	-0.51

Table S2. The T_1 diagnostic value, zero-point energy (ZPE), potential barriers, reaction heat, Gibbs free energy for the transition states, intermediates and products of the NO_3 + $CH{\equiv}CCH_2OH$ reactions in gaseous and aqueous phase. Units of $\Delta E_{(gas)}$, $\Delta H_{(gas)}$, $\Delta G_{(gas)}$, $\Delta E_{(aq)}$ and $\Delta G_{(aq)}$ are kcal/mol.

Species	ZPE	T_1	$\Delta E_{(gas)}$	$\Delta H_{(gas)}$	$\Delta G_{(gas)}$	$\Delta E_{(aq)}$	$\Delta G_{(aq)}$
$CH{\equiv}CCH_2OH + NO_3$	45.00	0.011 0.023	0.00	0.00	0.00	0.00	0.00
COMP1	46.56	0.023	25.82	25.84	35.19	19.88	29.25
IM1	48.53	0.028	-16.05	-16.77	-4.76	-15.98	-4.69
IM2	48.80	0.026	-15.85	-16.45	-5.40	-16.41	-5.36
IM3	47.86	0.021	-26.38	-27.34	-14.84	-25.26	-13.73
IM4	48.60	0.025	-48.61	-49.55	-36.87	-47.80	-36.07
IM5	48.19	0.021	-24.85	-25.78	-14.02	-24.06	-13.22
H-TS1	45.66	0.034	4.86	4.19	15.66	5.00	15.68
H-TS2	45.48	0.026	25.98	25.54	36.12	21.64	37.79
H-TS3	43.18	0.040	9.94	9.31	20.66	10.56	31.28
TS1	47.26	0.029	4.76	4.14	15.52	4.53	15.76
TS2	46.82	0.030	8.22	7.92	17.77	—	—
TS3	47.79	0.024	8.01	7.08	19.50	7.59	19.07
TS4	45.10	0.035	21.23	21.36	31.19	—	—
TS5	45.27	0.030	0.96	-0.29	12.84	2.15	14.03
TS6	45.51	0.029	15.32	14.25	27.04	16.17	27.89
TS7	42.97	0.026	-3.76	-4.50	7.71	-2.54	8.94
TS9	43.01	0.036	-2.39	-3.10	9.22	-1.95	9.65
TS8	47.36	0.030	-39.88	-40.78	-28.37	-39.81	-28.30
TS10	46.72	0.042	-3.12	-3.40	6.24	-3.32	6.34
TS11	45.76	0.026	20.17	19.22	31.32	17.82	28.97

TS12	45.73	0.028	15.53	14.48	26.66	16.66	27.79
TS13	43.40	0.036	-3.64	-4.33	7.20	-4.02	6.82
P1:(CH_2OH + HCCO + NO_2)	40.47	0.014 0.024 0.024	11.96	13.33	1.14	11.41	0.58
P2:(CH_2CONO_2CHO + H)	42.36	0.018	-11.89	-11.66	-6.08	-11.82	-6.02
P3:($CH_2COHCHO$ + NO_2)	47.22	0.015 0.024	-85.94	-86.41	-85.00	-85.15	-84.21
P4:($CHCOCH_2OH$ + NO_2)	44.80	0.019 0.024	-3.12	-2.84	-3.18	-5.92	-5.99
P5:(CHOCHCHOH + NO_2)	47.27	0.016 0.024	-81.40	-81.64	-80.76	-83.01	-82.36
P6:($CHONO_2CHCHO$ + H)	42.60	0.018	-11.49	-11.15	-6.67	-11.25	-6.43
h-P1: (CHCCHOH + HNO_3)	46.05	0.032 0.018	-18.82	-18.94	-18.98	-21.16	-21.33
h-P2: ($CCCH_2OH$ + HNO_3)	46.04	0.062 0.018	32.15	31.94	31.82	27.74	27.42
h-P3: ($CHCCH_2O$ + HNO_3)	45.44	0.018 0.018	2.19	1.85	2.10	-0.22	-0.31

Table S3 The harmonic vibrational frequencies (imaginary frequency is suffixed with *i*), the moment of inertia (I_a, I_b and I_c), rotational constants (GHZ) and the number of imaginary frequencies of all the species in the NO_3 + $CH{\equiv}CCH_2OH$ reactions in gaseous.

Species	Frequencies (cm^{-1})	I_a, I_b, I_c (amu $bohr^2$)	Rotational constants (GHZ)	the number of imaginary frequencies
$CH{\equiv}CCH_2OH$	198, 280, 349, 557, 663, 708, 913, 990, 1043, 1213, 1347, 1412, 1490, 2214, 2997, 3079, 3475, 3828	54.77812, 387.34460, 427.75128	32.94639, 4.65927, 4.21914	0
NO_3	282, 285, 800, 1106, 1110, 1130	130.43940, 130.53852, 260.97792	13.83586, 13.82535, 6.91530	0
COMP1	40, 49, 72, 87, 96, 197, 221, 225, 349, 546, 640, 692, 783, 856, 897, 959, 976, 1073,1214, 1226, 1234, 1404, 1428, 1511, 1705, 2003, 2371, 2933, 2949, 3828	277.94312, 2596.55844, 2765.93259	6.49320, 0.69505, 0.65249	0
IM1	60, 67, 103, 184, 238, 313, 344, 423, 487, 545, 669, 732,741, 756, 809, 883, 991, 1035,1094, 1211, 1340, 1351, 1406, 1491, 1682, 1754, 3002,3119, 3282, 3821	531.66389, 1231.62788, 1424.90544	3.39452, 1.46533, 1.26657	0
IM2	33, 51, 88, 154, 209, 226, 306, 438, 524, 585, 699, 748, 801, 828, 910, 988, 1012, 1054, 1232, 1240, 1304,1344, 1423, 1474,1738, 1762, 2929, 2989, 3197, 3835	317.38322, 2077.96372, 2162.57462	5.68632, 0.86851, 0.83453	0
IM3	67, 81, 85, 192, 261, 392, 415, 440, 560,613, 677, 738,783, 819, 878, 960, 965, 1081, 1151, 1184, 1327, 1349, 1374, 1406, 1711, 1749, 2880, 1711, 1749, 2880	412.66753, 1412.36698, 1560.59436	4.37335, 1.27781, 1.15644	0
IM4	56, 72, 192, 220, 254, 386, 420, 474, 511, 548, 634, 685, 715, 738, 766, 803, 919, 949, 1170, 1258, 1283, 1170, 1258, 1283, 1532, 1769, 3168, 3227, 3270, 3750	567.89069, 1101.69041, 1387.73374	3.17797, 1.63816, 1.30050	0

IM5	29, 60, 89, 167, 256, 337,450, 528, 572, 627, 730, 755, 766, 825, 951, 977, 1062, 1073, 1150, 1234, 1315, 1323, 1358, 1415, 1701, 1754, 2846, 2945, 3181, 3223	311.70464, 1964.54065, 2136.26139	5.78991, 0.91866, 0.84481	0
TS1	316*i*, 51, 69, 109, 148, 200, 254, 310, 425, 565, 584, 632,674, 686., 788, 869, 911, 985, 1067, 1212, 1298, 1353, 1411, 1482,1611, 2004, 3020, 3088, 3440, 3797	562.12058, 1286.86034, 1508.11070	3.21059, 1.40244, 1.19669	1
TS2	281*i*, 24, 42, 67, 119, 166, 183, 221, 341, 556, 605, 678,709, 785, 843, 891, 921, 972, 1063, 1227, 1248, 1295, 1432, 1467,1591, 2078, 2960, 2989, 3431, 3833	380.75933, 2179.54336, 2222.15450	4.73985, 0.82804, 0.81216	1
TS3	353*i*, 47, 98, 108, 188, 280, 287, 398, 429, 562, 686, 695, 719, 752, 787, 904, 959, 1035, 1068, 1130, 1216, 1361, 1410, 1470, 1534, 1995, 3009, 3074, 3417, 3795	457.50953, 1281.51596, 1653.32221	3.94471, 1.40829, 1.09158	1
TS4	381*i*, 39, 65, 83, 109, 146, 222, 276, 313,380, 448, 468, 517, 535, 583, 653, 785, 901, 1085, 1089, 1200, 1353, 1375, 1493, 1824, 1956, 3113, 3255, 3457, 3807	558.10155, 1460.61181, 1956.48968	3.23371, 1.23561, 0.92244	1
TS5	1915*i*, 60, 74, 123, 234, 375, 392, 446, 540, 623, 667, 723,739, 796, 808, 888, 974, 1027, 1047, 1182, 1194, 1329, 1364, 1499, 1641, 1780, 1805, 3017, 3059, 3249	348.48926, 1479.13211, 1580.17955	5.17876, 1.22014, 1.14211	1
TS6	1983*i*, 57, 70, 175, 209, 257, 374, 411, 467, 578, 640, 685,733, 771, 807, 856, 927, 973,1114, 1142, 1230,1270, 1348, 1420, 1627, 1762, 1805, 3139, 3173, 3799	510.74942, 1278.42481, 1454.41234	3.53352, 1.41169, 1.24087	1
TS7	770*i*, 60, 78, 118, 192, 267, 330, 392, 418, 442, 498, 600, 667, 737, 774, 815, 896, 970, 984, 1014, 1202, 1345, 1389, 1403, 1659, 1698, 1762, 2914, 3161, 3262,	434.51565, 1357.97800, 1515.62547	4.15346, 1.32899, 1.19076	1
TS8	516*i*, 62, 63, 130, 245, 251, 335, 354, 427, 335, 354, 427, 683,	580.10281, 1194.37439,	3.11107, 1.51103, 1.26608	1

	771, 781, 921, 933, 976, 1215, 1254, 1285,1346, 1375, 1473, 1545, 1777, 3161,3210, 3267, 3547	1425.45255		
TS9	999*i*, 73, 91, 153, 160, 193, 277, 366, 461, 476, 523, 623,679,738, 752, 814, 902, 950, 966, 987, 1265, 1356, 1370, 1430, 1639, 1654, 1772, 2983, 3160, 3257	584.13969, 1003.57795, 1299.13055	3.08957, 1.79831, 1.38919	1
TS10	283*i*, 24, 29, 53, 139, 157, 212, 308, 322, 372, 461, 679, 747, 885, 932, 954, 1056, 1194, 1220, 1226, 1349, 1369, 1406, 1461, 1511, 1783, 2944, 2971, 3069, 3839	429.98487, 1967.91452, 2105.26419	4.19722, 0.91708, 0.85725	1
TS11	1488*i*, 29, 75, 144, 218, 231, 331, 422, 472, 516, 618, 673, 715, 736, 800, 938, 1002, 1021, 1072, 1208, 1252,1311, 1353, 1431, 1530, 1738, 2080, 3039, 3227, 3813	295.74194, 2050.48452, 2220.1595	6.10242, 0.88015, 0.81289	1
TS12	2092*i*,35, 73, 92, 169, 251, 374, 418, 589,607, 714, 738, 790, 814, 865, 904, 980, 1033, 1071, 1126, 1283, 1320, 1369, 1498, 1750, 1778, 1982, 3042, 3090, 3219	248.98601, 2104.25302, 2257.22994	7.24836, 0.85766, 0.79954	1
TS13	818*i*, 25, 89, 115, 130, 273, 309, 382, 404, 471, 564, 574, 720, 782, 785, 817, 970, 1001, 1023, 1140, 1233, 1323, 1366, 1420, 1633, 1678, 1778, 2930, 3192, 3217	265.05926, 2046.45843, 2280.73425	6.80882, 0.88189, 0.79130	1
H-TS1	235*i*, 45, 62, 117, 140, 209, 219, 344, 479, 570, 599, 683, 686, 711, 794, 866, 934, 958, 1119, 1206, 1256, 1306, 1348, 1418, 1514, 1909, 2180, 3085, 3467, 3704	517.47721, 1655.24592, 1822.18170	3.48758, 1.09032, 0.99043	1
H-TS2	264*i*, 46, 56, 77, 101, 180, 211, 219, 345, 539, 582, 696, 784, 854, 907, 968, 1062, 1073, 1085, 1221, 1231, 1410,1434, 1512, 1611, 1838, 2032, 2938, 2956, 3828	269.47381, 2535.43166, 2694.46984	6.69728, 0.71181, 0.66979	1
H-TS3	1550*i*, 41, 63, 98, 140, 210, 252, 299, 442, 566, 688, 695,716, 758, 792, 797, 920, 1000, 1086, 1138, 1171, 1266, 1301, 1346,	493.66831, 1661.01040, 1826.68558	3.65578, 1.08653, 0.98799	1

	1517, 1605, 2188, 2620, 3011, 3467			
$CHONO_2CHCHO$	21, 103, 118, 142, 275, 379, 401, 567, 572, 719, 784, 791, 816, 980, 1009, 1023, 1154, 1235, 1326, 1382, 1438, 1665, 1754, 1782, 2944, 3190, 3213	247.38772, 2017.65178, 2265.03938	7.29519, 0.89448, 0.79678	0
CH_2CONO_2CHO	72, 91, 167, 185, 277, 364, 459, 517, 619, 683, 735, 760,814, 893, 969, 976, 1015, 1265, 1359, 1375, 1435, 1681, 1778, 1787, 2928, 3158, 3254	553.34506, 999.98173, 1267.99531	3.26151, 1.80477, 1.42330	0
CHOCHCHOH	188, 206, 256, 420, 445, 750, 845, 990, 992, 1026, 1170, 1249, 1341, 1366, 1428, 1667, 1763, 2904, 3161, 3183, 3843	86.54011, 662.25077, 748.79088	20.85439, 2.72516, 2.41021	0
$CH_2COHCHO$	201, 282, 410, 525, 559, 681, 734, 892, 895, 981, 1001, 1256, 1366, 1397, 1446, 1707, 1745, 2975, 3164, 3258, 3682	176.79662, 397.34630, 574.14289	10.20801, 4.54199, 3.14337	0
CHCCHOH	216, 322, 354, 423, 595, 604, 714, 985, 1205, 1293, 1439, 2038, 3228, 3467, 3807	37.52641, 382.24006, 419.76647	48.09256, 4.72149, 4.29939	0
$CCCH_2OH$	190, 206, 314, 517, 853, 903, 1056, 1211, 1225, 1402, 1426, 1645, 2940, 2966, 3826	48.84067, 367.93856, 403.22265	36.95161, 4.90501, 4.47579	0
$CHCCH_2O$	208, 290, 537, 572, 676, 708, 912, 1049, 1138, 1310, 1369, 2215, 2902, 2903, 3473,	43.31309, 384.96493, 417.48800	41.66734, 4.68807, 4.32286	0
CH_2OH	405, 530, 1050, 1198, 1350, 1480, 3126, 3273, 3843	9.32332, 60.44413, 69.21301	193.57276, 29.85801, 26.07517	0
HNO_3	460, 586, 648, 773,896, 1319, 1348, 1755, 3729	138.54720, 150.29389, 288.84109	13.02618, 12.0080, 6.24821	0
NO_2	764, 1391, 1702	7.43909, 138.23124, 145.67032	242.60243, 13.05596, 12.38922	0

Table S4 The Cartesian coordinates at the B3LYP/6-311++G(d,p) level of all the species in the NO_3 + $CH{\equiv}CCH_2OH$ reactions in gaseous.

Species		Coordinates(Atom, X, Y, Z)		
$CH{\equiv}CCH_2OH$	C	0.77603300	0.15430300	-0.00237400
	C	1.91938000	-0.21748700	-0.01353000
	H	2.92967000	-0.54674300	-0.03233400
	C	-0.62100800	0.58915300	0.03498300
	H	-0.82327600	1.26437400	-0.79956100
	H	-0.79858800	1.15148600	0.96151200
	O	-1.55319100	-0.48277000	-0.09868300
	H	-1.32871200	-1.16276900	0.54538100
NO_3	N	0.00000000	0.00000000	-0.00013300
	O	0.00000000	-1.06856200	-0.61713000
	O	0.00000000	1.06856200	-0.61713000
	O	0.00000000	0.00000000	1.23437600
COMP1	C	1.59081500	0.47837500	0.22548900
	C	0.47880700	1.05064700	0.04966100
	H	-1.12954700	1.31796000	-0.15181200
	C	2.88579500	-0.08680600	0.49872800
	H	2.71467000	-0.96720200	1.14432200
	H	3.44728500	0.63608100	1.11564900
	N	-2.19919600	-0.23435200	-0.01792700
	O	-3.28258700	-0.75026700	-0.04155700
	O	-1.12280400	-0.81928100	0.17595400
	O	-2.14864100	1.10051700	-0.22049600
	O	3.58083100	-0.42560200	-0.68652500
	H	4.41507200	-0.84260500	-0.44494700
IM1	C	-0.77803100	0.67192700	-0.13582400
	C	-0.98105600	1.94689300	-0.34144000
	H	-0.54200600	2.79446300	-0.84075600
	C	-1.65227300	-0.28057300	0.63671600
	H	-2.48520600	0.26995600	1.07246300
	H	-1.07066500	-0.72368300	1.45618000
	N	1.51368800	-0.15301700	0.06919900
	O	1.47346800	0.31615400	1.17059300
	O	2.36148600	-0.76836300	-0.49926600
	O	0.31603900	0.04971200	-0.79271500
	O	-2.21673900	-1.28799000	-0.19222900
	H	-1.50380800	-1.77521000	-0.62005100

IM2	C	-1.41207900	0.64104000	-0.43332200
	C	-0.12153000	0.81652500	-0.55786500
	H	0.36894200	1.76766100	-0.72073800
	C	-2.42122900	-0.41126700	-0.29179000
	H	-1.89510900	-1.36824300	-0.12798900
	H	-2.98358500	-0.50171700	-1.23229700
	N	1.98891800	-0.12281300	0.14850900
	O	2.67570200	-1.09806000	0.09330300
	O	2.17257800	0.94550000	0.66534700
	O	0.72528400	-0.30861300	-0.56842600
	O	-3.28757400	-0.10557700	0.79748500
	H	-3.97156400	-0.78179700	0.83765900
IM3	C	-0.70876100	0.51467500	-0.13715900
	C	-1.21514500	1.61676400	0.39756100
	H	-0.61740700	2.51379300	0.49161700
	C	-1.44203000	-0.79082700	-0.36052500
	H	-0.94310700	-1.61295400	0.19477200
	H	-1.34339500	-1.10973100	-1.41695500
	N	1.60950000	-0.15976500	0.09054200
	O	1.25426100	-0.67079900	1.11774600
	O	2.67490700	-0.11860500	-0.44070800
	O	0.57652400	0.55781700	-0.69026200
	O	-2.74588300	-0.81151200	0.00943700
	H	-2.24544600	1.62837400	0.72780500
IM4	C	-0.88649800	0.57522600	-0.21686300
	C	-0.96496700	1.95370100	-0.20942600
	H	-0.15416200	2.55398200	-0.59560200
	C	-1.84980300	-0.32554900	0.21881200
	H	-1.83785800	2.45113300	0.19068100
	H	-2.79141700	-0.00569200	0.64152800
	N	1.44858300	-0.09878300	0.10166200
	O	1.33384700	0.35798800	1.19811000
	O	2.36595000	-0.61554500	-0.45672700
	O	0.23698500	-0.03655700	-0.79643900
	O	-1.71748300	-1.66337000	0.13560300
	H	-0.90343200	-1.86834600	-0.34775200
IM5	C	-1.49131300	0.79563100	-0.26121300
	C	-0.17068900	0.90017700	-0.37369600
	H	0.37268300	1.83122800	-0.45391400
	C	-2.25867500	-0.49114000	-0.12761100
	H	-1.62843000	-1.31850800	0.24220300
	H	-2.58083100	-0.85948200	-1.12771100
	N	1.94039500	-0.15545700	0.10005700

	O	2.55032000	-1.17066900	-0.03914300
	O	2.24532500	0.89243600	0.59871500
	O	0.59291700	-0.25397500	-0.47595100
	O	-3.40694600	-0.40560800	0.60272500
	H	-2.07505400	1.70948200	-0.27663000
TS1	C	-1.17668900	0.79012400	-0.02051600
	C	-1.11265900	1.95408000	-0.41657200
	H	-0.90503600	2.92155000	-0.81187100
	C	-1.75556400	-0.40188900	0.63031100
	H	-2.72392700	-0.11937600	1.04998700
	H	-1.10040200	-0.69754500	1.45862200
	N	1.53848200	-0.08471500	0.05809200
	O	1.41935900	0.36162800	1.17968700
	O	2.51370700	-0.61582000	-0.43171600
	O	0.48147500	-0.02136200	-0.79425100
	O	-1.99113600	-1.46170200	-0.27226200
	H	-1.15777800	-1.66746300	-0.71438100
TS2	C	-1.47852000	0.65309300	-0.32450900
	C	-0.42293100	1.27591000	-0.30116900
	H	0.24434100	2.10032900	-0.19691000
	C	-2.58827600	-0.27241900	-0.44479100
	H	-2.20108900	-1.17557200	-0.94399400
	H	-3.34546200	0.16785700	-1.11034300
	N	2.01276500	-0.16409000	0.09623000
	O	2.86246600	-0.98403100	-0.19875300
	O	2.00247300	0.57543900	1.05953000
	O	1.00272300	-0.10941800	-0.79050800
	O	-3.12201300	-0.56416100	0.83785600
	H	-3.81397800	-1.22611300	0.73544700
TS3	C	-0.96218100	0.81001700	0.11427300
	C	-0.22437800	1.77390600	-0.15776200
	N	1.50655200	-0.30153800	0.04475500
	O	1.67255700	0.94615400	-0.15025200
	O	2.41695600	-1.09187200	-0.06535100
	O	0.32480600	-0.71508500	0.37532400
	H	0.13267100	2.74701100	-0.40923400
	C	-2.18522000	0.03105500	0.37280300
	H	-2.15801400	-0.32358700	1.41114500
	H	-3.04483400	0.69921800	0.26912600
	O	-2.37099700	-1.02739400	-0.54223800
	H	-1.59159400	-1.59616500	-0.50007400
TS4	C	-0.41138000	0.94152400	0.08819800
	C	-0.36274600	2.16653200	-0.05026000

	H	-0.59897000	3.19173200	-0.19994700
	C	-2.47222400	-0.04961700	0.29999900
	H	-3.05317400	0.78013300	-0.07803200
	H	-2.36192300	-0.17537600	1.37227700
	N	1.75751500	-0.35711600	-0.00643200
	O	2.30113000	0.66305500	-0.25313100
	O	2.10312100	-1.48222200	0.13177600
	O	0.06654600	-0.25216700	0.21851500
	O	-2.56952000	-1.15249700	-0.46895000
	H	-2.02065300	-1.85666800	-0.10257600
TS5	C	-0.66565000	0.42400900	-0.15182800
	C	-1.40308400	1.29004500	0.53248700
	H	-1.27508500	2.28501000	0.93168900
	C	-1.45128000	-0.80974300	-0.52136200
	H	-1.02921900	-1.72320200	-0.08996800
	H	-1.52242300	-0.91479900	-1.61025900
	N	1.68741700	-0.12395500	0.09534500
	O	1.33110100	-0.81473100	1.00265600
	O	2.75074100	0.07722000	-0.39309600
	O	0.60339000	0.68231300	-0.60107500
	O	-2.73045600	-0.53693300	0.04097400
	H	-2.50331200	0.53185400	0.54966100
TS6	C	-0.72036800	0.64487100	-0.06877700
	C	-1.46490900	1.72821500	0.12572700
	H	-1.34081500	2.79484300	-0.03412400
	C	-1.59726900	-0.45922200	0.42479000
	H	-2.37494100	0.67812300	0.62130100
	H	-1.41180400	-0.85940400	1.41901600
	N	1.57371100	-0.10072000	0.07090100
	O	1.32014700	-0.34857600	1.21518000
	O	2.55488100	-0.26881800	-0.58133500
	O	0.48810700	0.55103800	-0.72448000
	O	-2.00796100	-1.46496700	-0.41764000
	H	-2.03453700	-1.14112500	-1.32673700
TS7	C	-0.71433500	0.53938500	-0.12687300
	C	-1.24839600	1.62366500	0.43021200
	H	-0.67536900	2.53393100	0.54856300
	C	-1.44511000	-0.75691500	-0.31511600
	H	-0.82593400	-1.58435200	-0.71397500
	H	-1.69287700	-0.46090300	-2.13423600
	N	1.58695600	-0.16560100	0.10167200
	O	1.20560000	-0.70491400	1.10183700
	O	2.65638100	-0.11555600	-0.41644000

	O	0.56469200	0.59967600	-0.67132900
	O	-2.57494400	-0.94952700	0.09905200
	H	-2.28130400	1.59629000	0.75364300
TS8	C	-0.96109100	0.56882200	-0.23876300
	C	-1.16374900	1.93182200	0.03354300
	H	-0.50152000	2.67302200	-0.39071000
	C	-1.81463900	-0.43286400	0.24567100
	H	-1.98597600	2.25647100	0.65723600
	H	-2.71265800	-0.24718700	0.82192000
	N	1.56056900	-0.08277600	0.12292600
	O	1.31986300	-0.03369400	1.28842100
	O	2.55625700	-0.21952700	-0.50658200
	O	0.04482200	0.10690700	-0.96941100
	O	-1.58408400	-1.70238600	-0.01416300
	H	-0.78181500	-1.71995500	-0.57775700
TS9	C	-1.01128800	0.51888100	-0.11798200
	C	-1.76670600	1.57934100	0.19277700
	H	-1.39102500	2.58779500	0.08101100
	C	-1.50044200	-0.86413700	-0.02391400
	H	-2.78631200	1.44113400	0.53053600
	H	-2.50466300	-0.97519400	0.41662800
	N	1.35976600	0.16923500	0.11269600
	O	1.10448200	-0.14730200	1.23845400
	O	2.37325300	0.16120600	-0.50737800
	O	0.23049700	0.71996800	-0.69145600
	O	-0.85012900	-1.83787100	-0.39118900
	H	-0.03056600	-2.81089700	0.69022200
TS10	C	-1.40595000	0.66645700	0.42520000
	C	-0.18261000	1.26286500	0.50465600
	H	0.07113000	1.88443900	1.36771200
	C	-2.12315700	-0.18462600	-0.53010300
	H	-1.42569500	-0.95384000	-0.90141400
	H	-2.41749200	0.43261000	-1.39396200
	N	1.98653200	-0.34406800	0.00865500
	O	2.88680000	-0.39696300	-0.75881900
	O	1.67131200	-0.95575900	0.97890600
	O	0.68036100	1.10766300	-0.44505100
	O	-3.25749300	-0.76778000	0.10142700
	H	-3.71120400	-1.32021400	-0.54314400
TS11	C	-1.42463300	0.79980500	-0.02252700
	C	-0.11795900	0.90895600	-0.36869900
	H	0.39667400	1.82666900	-0.61119800
	C	-2.30758800	-0.27271700	-0.22897500

	H	-2.06525400	-1.14300800	-0.84704100
	H	-2.41254300	0.86822200	-0.90489200
	N	1.99694100	-0.17686500	0.09984200
	O	2.58319500	-1.21393400	-0.00342200
	O	2.33904800	0.88601600	0.54069900
	O	0.63546400	-0.26038200	-0.46209900
	O	-3.40534100	-0.39814300	0.57421500
	H	-4.01530900	-1.03854800	0.19030700
TS12	C	1.46357100	0.28626800	0.13860800
	C	0.22457700	0.58166900	0.46936700
	H	-0.11457800	1.54842600	0.81360500
	C	2.40343000	-0.74898300	-0.29081300
	H	2.31067600	-1.07917400	-1.32850400
	H	2.51947300	-1.60288100	0.38068800
	N	-2.03725700	-0.03525000	-0.08358100
	O	-2.82052200	-0.93279300	-0.04670500
	O	-2.14361000	1.09966500	-0.45823300
	O	-0.72514900	-0.43817400	0.45485700
	O	3.48923600	0.22574800	-0.12379200
	H	2.59612400	1.03108300	0.20729200
TS13	C	1.52070700	0.80809200	0.06360000
	C	0.18242900	0.84511300	0.09048500
	H	-0.39938600	1.75631900	0.13329400
	C	2.33891500	-0.41792600	-0.05155600
	H	1.78370200	-1.36721300	-0.16737900
	H	2.22082600	-0.82046100	1.72815400
	N	-2.01359700	-0.15725100	-0.03199900
	O	-2.55355900	-1.21591100	-0.02362900
	O	-2.43548100	0.96014700	-0.10968600
	O	-0.54164900	-0.31810800	0.08384900
	O	3.55336500	-0.37975400	-0.22338300
	H	2.05632200	1.74944700	0.09754700
H-TS1	C	-2.11808500	0.52899600	0.08822500
	C	-2.64669000	1.53104000	-0.32419100
	H	-3.12417900	2.40663400	-0.69429800
	C	-1.44863600	-0.64376700	0.59830800
	H	-1.93175900	-1.06505400	1.48287900
	H	-0.40559700	-0.26134200	0.97711400
	N	1.72728200	0.15981300	-0.06081800
	O	1.12328800	-0.21887300	-1.06064700
	O	2.88000000	0.54341100	-0.03727600
	O	1.11158100	0.16515700	1.09566300
	O	-1.19894600	-1.66407500	-0.30683600

	H	-0.67636500	-1.30150700	-1.04125900
H-TS2	C	1.54524400	0.45221800	0.23392300
	C	0.41958900	0.98343000	0.06022300
	H	-1.04976500	1.30661200	-0.14161100
	C	2.85924200	-0.07568700	0.50068500
	H	2.72109200	-0.95819200	1.15019300
	H	3.40780600	0.66647100	1.10517500
	N	-2.17267000	-0.21359400	-0.02302900
	O	-3.24318600	-0.75706100	-0.04507500
	O	-1.08557800	-0.80576000	0.17764200
	O	-2.12121900	1.10218300	-0.22209400
	O	3.54854800	-0.40012900	-0.69314600
	H	4.39658300	-0.79336000	-0.46016400
H-TS3	C	2.22747800	-0.44692500	0.01905900
	C	2.76933900	-1.43358300	-0.40816700
	H	3.24869000	-2.30093800	-0.79490800
	C	1.58167100	0.73605300	0.56560200
	H	2.26387600	1.34324500	1.17536800
	H	0.79591200	0.36664600	1.29387800
	N	-1.72241700	-0.20778500	0.04942100
	O	-1.11460900	-0.31585900	1.11984200
	O	-2.80710100	-0.68650400	-0.17797500
	O	-1.16222000	0.47427600	-0.93699000
	O	0.87958800	1.52153700	-0.30359100
	H	-0.08775400	0.96467000	-0.68953500
$CHONO_2CHCHO$	C	-1.56803700	0.78760700	-0.00006300
	C	-0.22810000	0.82408200	0.00035000
	H	0.35116500	1.73854300	0.00062600
	C	-2.37596200	-0.43864000	-0.00051200
	H	-1.81824100	-1.39335100	-0.00157300
	N	1.98262400	-0.15595500	-0.00008300
	O	2.52761900	-1.21121100	0.00009000
	O	2.39835600	0.96584000	-0.00044100
	O	0.50340300	-0.33131100	0.00053800
	O	-3.58909000	-0.42618000	0.00016500
	H	-2.10100700	1.73108800	0.00006900
CH_2CONO_2CHO	C	1.01642700	-0.46279400	-0.13366800
	C	1.80409500	-1.50718300	0.12908200
	H	1.46003100	-2.52341100	-0.01271700
	C	1.47602200	0.94250400	0.02662400
	H	2.82255600	-1.34813600	0.46201000
	H	2.49480700	1.03956500	0.45010800
	N	-1.35768400	-0.14233200	0.11831600

	O	-1.11032100	0.09790500	1.26343500
	O	-2.36285600	-0.08806900	-0.51154700
	O	-0.22115400	-0.66261000	-0.70743100
	O	0.81272300	1.90191800	-0.27693600
CHOCHCHOH	C	-0.02473200	0.71575500	-0.00004500
	C	-1.45646400	0.40670100	0.00008200
	H	-2.12014600	1.29503500	0.00042500
	C	0.88252400	-0.27334900	0.00008400
	H	0.56391100	-1.31232600	0.00024400
	H	0.28843900	1.75370600	-0.00016200
	O	-1.93921000	-0.71116900	-0.00010700
	O	2.20929800	-0.03479200	-0.00011300
	H	2.69912200	-0.86337700	0.00052400
$CH_2COHCHO$	C	0.50750200	0.01474700	0.00003200
	C	1.66922600	-0.65274000	-0.00023400
	H	2.62292900	-0.14177400	-0.00053200
	C	-0.78509400	-0.70145200	0.00029800
	H	1.66144400	-1.73447900	0.00012600
	H	-0.74030600	-1.80403800	0.00099400
	O	0.41709400	1.36227800	0.00019500
	O	-1.83750900	-0.09517700	-0.00033200
	H	-0.53055200	1.58014900	-0.00007000
CHCCHOH	C	0.72993800	0.16034200	-0.00014100
	C	1.90008100	-0.19076300	0.00024400
	H	2.92108000	-0.48467200	-0.00082200
	C	-0.59014100	0.53609900	0.00010900
	H	-0.91998300	1.56404000	-0.00021400
	O	-1.62169000	-0.35732300	-0.00004200
	H	-1.26684900	-1.25485100	0.00009600
$CCCH_2OH$	C	0.87941100	0.07282500	-0.13915200
	C	2.06674900	-0.29367300	0.07804000
	C	-0.47755400	0.54425200	0.02419500
	H	-0.66794200	1.27893200	-0.77727200
	H	-0.52984200	1.10230000	0.97307300
	O	-1.41515000	-0.52035100	-0.01550700
	H	-2.29265700	-0.15885000	0.14975900
$CHCCH_2O$	C	0.73173600	0.11404000	0.00024600
	C	1.89756100	-0.17776400	-0.00002400
	H	2.92655700	-0.44453000	-0.00042200
	C	-0.68787900	0.48163000	-0.00002400
	H	-0.91842000	1.13274400	-0.86630500
	H	-0.91856300	1.13407800	0.86518300
	O	-1.59226000	-0.54121600	0.00004500

HCCO	C	0.00000000	0.00000000	-1.23902800
	H	0.00000000	0.00000000	-2.30089500
	C	0.00000000	0.00000000	0.01897200
	O	0.00000000	0.00000000	1.20265400
CH_2OH	C	0.68507700	0.02779300	0.05922500
	H	1.23590400	-0.88864600	-0.08991500
	H	1.11999500	0.99621300	-0.15801100
	O	-0.67044200	-0.12553900	-0.02133900
	H	-1.10283100	0.72998200	0.06329100
HNO_3	N	0.00000000	0.15625600	0.00000000
	O	-0.98240900	0.83466400	0.00000000
	O	1.16913700	0.46883500	0.00000000
	O	-0.26444200	-1.23577200	0.00000000
	H	0.62172100	-1.63560100	0.00000000
NO_2	N	0.00000000	0.00000000	0.32172200
	O	0.00000000	1.10001400	-0.14075300
	O	0.00000000	-1.10001400	-0.14075300

Table S5 The calculated overall ($k_{overall}$) and branching rate constants ($k_{H\text{-}TS1}$, $k_{H\text{-}TS3}$, k_{IM1}, k_{IM2}, k_{IM3}, k_{P2} and k_{P4}) of the $CH{\equiv}CCH_2OH + NO_3$ reaction at the temperature of 200-2000 K and the experimental values (cm^3 $molecule^{-1}$ s^{-1}).

T/K	$k_{H\text{-}TS1}$	$k_{H\text{-}TS3}$	k_{IM1}	k_{IM2}	k_{IM3}	k_{P2}	k_{p4}	$k_{overall}$
200	3.99×10^{-20}	2.62×10^{-25}	1.10×10^{-17}	1.23×10^{-20}	1.19×10^{-23}	2.38×10^{-27}	1.77×10^{-21}	1.11×10^{-17}
250	3.78×10^{-19}	5.86×10^{-24}	8.22×10^{-17}	4.65×10^{-19}	1.76×10^{-21}	4.12×10^{-24}	2.67×10^{-19}	8.43×10^{-17}
293	1.50×10^{-18}	5.94×10^{-23}	2.89×10^{-16}	3.25×10^{-18}	4.80×10^{-20}	5.93×10^{-22}	4.80×10^{-18}	3.06×10^{-16}
296	1.63×10^{-18}	6.90×10^{-23}	3.12×10^{-16}	3.61×10^{-18}	5.89×10^{-20}	8.06×10^{-22}	5.68×10^{-18}	3.31×10^{-16}
298	1.72×10^{-18}	7.61×10^{-23}	3.28×10^{-16}	3.87×10^{-18}	6.74×10^{-20}	9.86×10^{-22}	6.34×10^{-18}	3.48×10^{-16}
300	1.81×10^{-18}	8.39×10^{-23}	3.45×10^{-16}	4.14×10^{-18}	7.71×10^{-20}	1.20×10^{-21}	7.06×10^{-18}	3.67×10^{-16}
325	3.39×10^{-18}	2.68×10^{-22}	6.15×10^{-16}	8.69×10^{-18}	3.68×10^{-19}	1.23×10^{-20}	2.42×10^{-17}	6.75×10^{-16}
350	5.87×10^{-18}	7.72×10^{-22}	1.03×10^{-15}	1.54×10^{-17}	1.47×10^{-18}	9.49×10^{-20}	6.87×10^{-17}	1.18×10^{-15}
375	9.57×10^{-18}	2.02×10^{-21}	1.62×10^{-15}	2.39×10^{-17}	5.00×10^{-18}	5.67×10^{-19}	1.69×10^{-16}	1.95×10^{-15}
400	1.48×10^{-17}	4.83×10^{-21}	2.43×10^{-15}	3.34×10^{-17}	1.47×10^{-17}	2.71×10^{-18}	3.68×10^{-16}	3.12×10^{-15}
425	2.21×10^{-17}	1.07×10^{-20}	3.51×10^{-15}	4.29×10^{-17}	3.80×10^{-17}	1.07×10^{-17}	7.34×10^{-16}	4.87×10^{-15}
433	2.49×10^{-17}	1.37×10^{-20}	3.92×10^{-15}	4.59×10^{-17}	5.02×10^{-17}	1.59×10^{-17}	9.01×10^{-16}	5.60×10^{-15}
450	3.17×10^{-17}	2.23×10^{-20}	4.89×10^{-15}	5.18×10^{-17}	8.71×10^{-17}	3.54×10^{-17}	1.36×10^{-15}	7.45×10^{-15}
475	4.42×10^{-17}	4.37×10^{-20}	6.59×10^{-15}	5.93×10^{-17}	1.79×10^{-16}	1.02×10^{-16}	2.37×10^{-15}	9.34×10^{-15}
500	6.00×10^{-17}	8.12×10^{-20}	8.60×10^{-15}	6.52×10^{-17}	3.35×10^{-16}	2.56×10^{-16}	3.92×10^{-15}	1.12×10^{-14}
600	1.68×10^{-16}	6.40×10^{-19}	1.87×10^{-14}	7.46×10^{-17}	1.88×10^{-15}	3.93×10^{-15}	2.02×10^{-14}	1.67×10^{-14}
700	3.78×10^{-16}	3.14×10^{-18}	2.71×10^{-14}	7.04×10^{-17}	4.41×10^{-15}	2.14×10^{-14}	6.97×10^{-14}	3.44×10^{-13}
800	7.36×10^{-16}	1.12×10^{-17}	2.91×10^{-14}	6.29×10^{-17}	6.03×10^{-15}	6.44×10^{-14}	1.86×10^{-13}	1.60×10^{-12}
900	1.29×10^{-15}	3.22×10^{-17}	2.54×10^{-14}	5.56×10^{-17}	5.93×10^{-15}	1.38×10^{-13}	4.14×10^{-13}	7.35×10^{-12}
1000	2.11×10^{-15}	7.83×10^{-17}	1.96×10^{-14}	4.97×10^{-17}	4.79×10^{-15}	2.44×10^{-13}	8.15×10^{-13}	3.23×10^{-11}
1200	4.78×10^{-15}	3.29×10^{-16}	9.96×10^{-15}	4.13×10^{-17}	2.36×10^{-15}	5.62×10^{-13}	2.41×10^{-12}	5.00×10^{-10}
1400	9.31×10^{-15}	1.01×10^{-15}	5.11×10^{-15}	3.62×10^{-17}	1.07×10^{-15}	1.06×10^{-12}	5.63×10^{-12}	5.82×10^{-9}
1600	1.63×10^{-14}	2.52×10^{-15}	2.92×10^{-15}	3.31×10^{-17}	5.19×10^{-16}	1.77×10^{-12}	1.12×10^{-11}	5.29×10^{-8}
1800	2.64×10^{-14}	5.40×10^{-15}	1.87×10^{-15}	3.11×10^{-17}	2.83×10^{-16}	2.75×10^{-12}	1.99×10^{-11}	3.93×10^{-7}
2000	4.03×10^{-14}	1.04×10^{-14}	1.32×10^{-15}	2.97×10^{-17}	1.72×10^{-16}	3.95×10^{-12}	3.19×10^{-11}	2.46×10^{-6}

Table S6. The acute and chronic toxicity class (mg L^{-1}).

Classification	Acute toxicity[1]	Chronic toxicity[2]
Not harmful	LC_{50}>100 or EC_{50}>100	ChV>10
Harmful	10< LC_{50} <100 or 10< EC_{50} <100	1< ChV <10
Toxic	1< LC_{50} <10 or 1< EC_{50} <10	0.1< ChV <1
Very toxic	LC_{50}<1 or EC_{50}<1	ChV<0.1

[1]Criteria set by the European Union (described in Annex VI of Directive 67/548/EEC);

[2]Criteria set by the Chinese hazard evaluation guidelines for new chemical substances (HJ/T 154–2004).

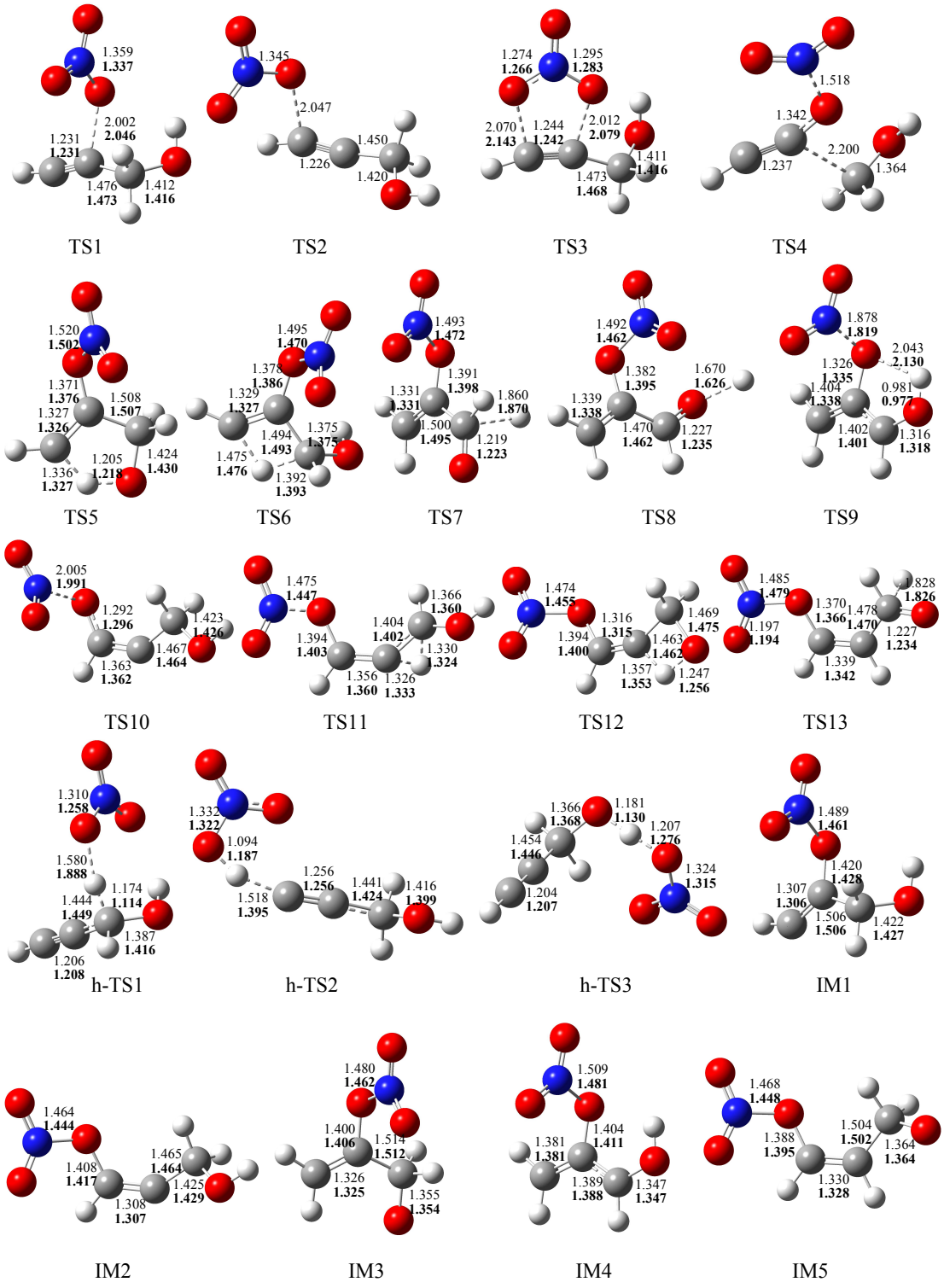

Fig S1. The optimized geometries for all the transition states and intermediates on the PESs involved in NO_3 + CH≡CCH_2OH reaction using B3LYP method. Bond distances are in Å. The first and bold values represents the gaseous phase and aqueous phase under the implicit water model (PCM), respectively.

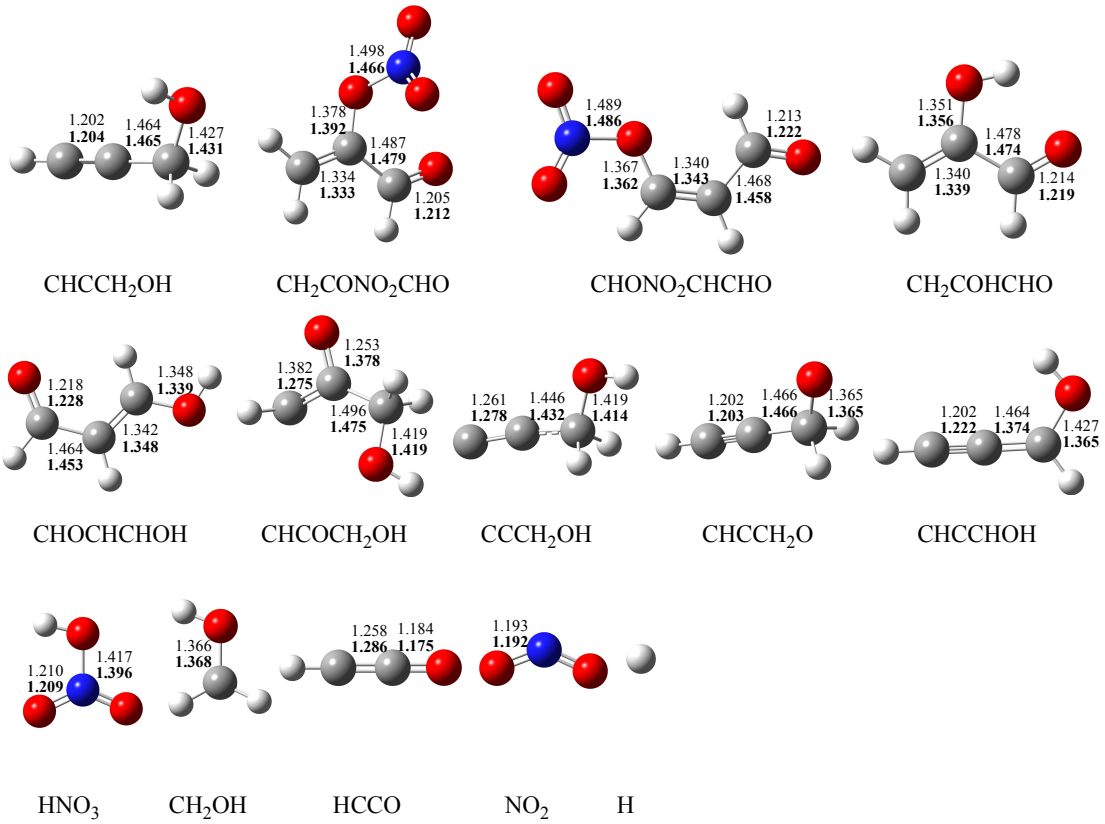

Fig S2. The optimized geometries for all products on the PESs involved in NO_3 + $CH{\equiv}CCH_2OH$ reaction using B3LYP method. Bond distances are in Å. The first and bold values represents the gaseous phase and aqueous phase under the implicit water model (PCM), respectively.