

**Supporting information
-for-**

**Atmospheric Chemistry of the Self-Reaction of HO₂ Radical:
Stepwise Mechanism Versus One-Step Process in the Presence of
(H₂O)_n (*n* = 1-3) Clusters**

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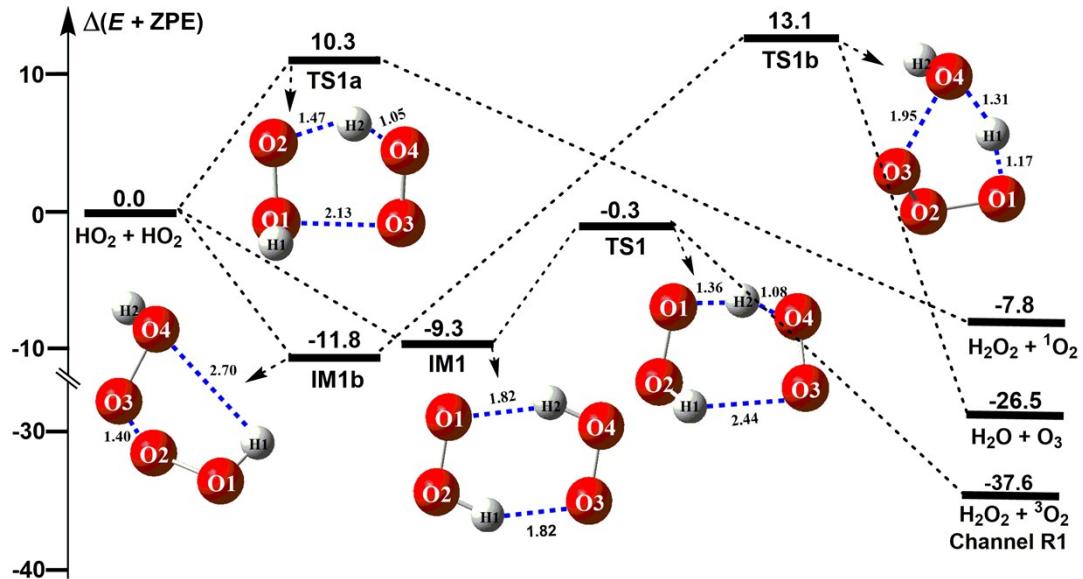


Fig. S1 Schematic energy diagrams for the dominant channel of $\text{H}_2\text{O}_2 + {}^3\text{O}_2$, $\text{H}_2\text{O}_2 + {}^1\text{O}_2$ and $\text{O}_3 + \text{H}_2\text{O}$ formations without water ($\text{kcal}\cdot\text{mol}^{-1}$)

The reaction between HO_2 and HO_2 on both singlet and triplet potential energy surfaces (PESs) have been investigated theoretically in previous studies,¹⁻³ where the channels of $\text{H}_2\text{O}_2 + {}^3\text{O}_2$ formation (triplet PES), $\text{H}_2\text{O}_2 + {}^1\text{O}_2$ formation (singlet PES) and $\text{O}_3 + \text{H}_2\text{O}$ formation (singlet PES) have been considered. Moreover, the channel of $\text{H}_2\text{O}_2 + {}^3\text{O}_2$ formation on the triplet potential energy surface has been identified as the most favorable channel.¹⁻³ In this study, we reinvestigated the channel of $\text{H}_2\text{O}_2 + {}^3\text{O}_2$ formation (reaction (1)) to determine the reliability of the theoretical methods used here and the catalytic effect of $(\text{H}_2\text{O})_n$ ($n = 1-3$). For comparison, the singlet channels of $\text{H}_2\text{O}_2 + {}^1\text{O}_2$ formation and $\text{O}_3 + \text{H}_2\text{O}$ formation have been involved in Fig. S1. As shown in Fig. S1, at the entrance of the channel of $\text{H}_2\text{O}_2 + {}^3\text{O}_2$ formation, the formation of six-member-ring hydrogen bonded intermediate IM has been identified via two hydrogen bonds, $\text{O}(1)\cdots\text{H}(2)$ (1.82 Å) and $\text{O}(3)\cdots\text{H}(1)$ (1.82 Å) with a bonding energy of 9.3 $\text{kcal}\cdot\text{mol}^{-1}$. After IM, the reaction goes through transition state TS to form $\text{H}_2\text{O}_2 + {}^3\text{O}_2$. From an energetic point of view, Fig. S1 and Table S1 show that at 298.15 K, TS was predicted to be 0.3 $\text{kcal}\cdot\text{mol}^{-1}$ below the $\text{HO}_2 + \text{HO}_2$ reactants at the CCSD(T)-F12/VTZP//M06-2X/aug-cc-pVTZ level of theory. For Reaction (1) without water, Table S1 lists its CVT/SCT rate constant. As shown in Table S1, tunneling slightly increases the rate constant, while the recrossing effects decrease the rate constant. For example, the rate constant is increased by 43% due to tunneling, while the rate constant is decreased to 70% because of recrossing effects at the M06-2X/aug-cc-pVTZ level and at 298.15 K (Table S1). It is noted that the tunneling and recrossing effects slightly depend on the temperature. Tunneling slightly increases with the decrease in temperature, while recrossing effects slightly

increases with the increase in temperature as listed in Table S1. Specifically, the calculated results using M06-2X/aug-cc-pVTZ indicate that, at 275 and 320 K, the rate constant is increased by 89% and 77% due to tunneling, while the rate constant is decreased to 15% and 18% due to recrossing effects, respectively. So, similar with previous investigations,³⁻⁵ the tunneling transmission coefficients are very large for the hydrogen atom transfer process. Thus, herein the computed CVT/SCT rate constants have been used to estimate the catalytic effect of $(\text{H}_2\text{O})_n$ ($n = 1-3$).

Table S1 Energy barriers (ΔE , 0 K) for the $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction at different theoretical methods with zero-point correction involved and unsigned error (UE) (in $\text{kcal}\cdot\text{mol}^{-1}$)

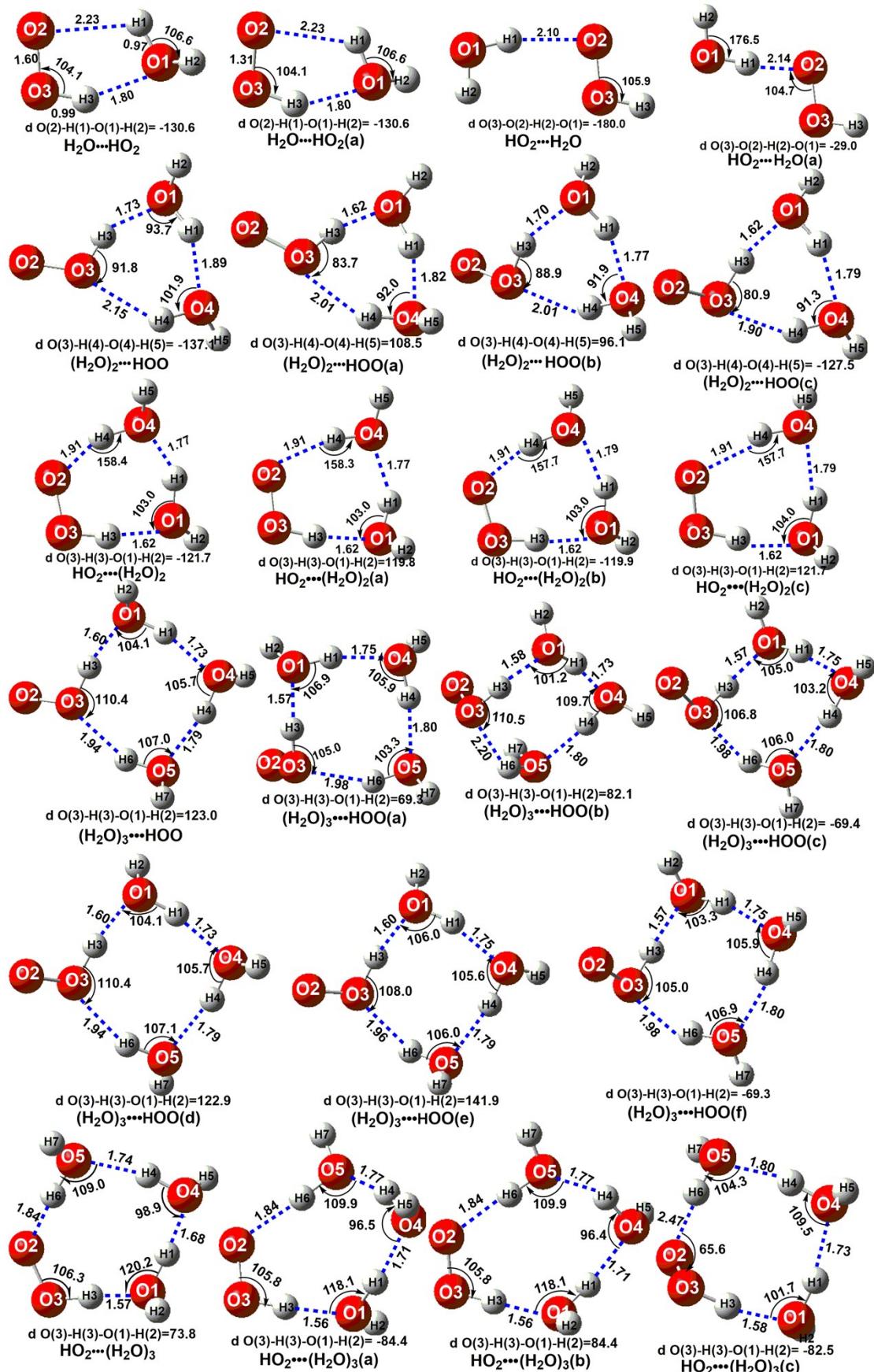
Methods	ΔE	UE
W3X-I//M06-2X/aug-cc-pVTZ	-1.2	0.00
W2X//M06-2X/aug-cc-pVTZ	-0.6	0.60
CCSD(T)-F12/VTZP//M06-2X/aug-cc-pVTZ	-0.3	0.90

Table S2 Rate constants ($\text{cm}^3 \cdot \text{molecules}^{-1} \cdot \text{s}^{-1}$) for the $\text{HO}_2 + \text{HO}_2$ reaction within the temperature range of 275.0-320.0 K

T/K	κ^{SCT}	I^{CVT}	$k_{\text{uni}}^{\text{CVT/SCT}}$	k_{R1}
275.0	271.89	0.15	6.89×10^8	1.72×10^{-11}
280.0	220.72	0.16	7.39×10^8	1.33×10^{-11}
290.0	148.95	0.16	8.47×10^8	8.22×10^{-12}
298.15	110.43	0.17	9.43×10^8	5.70×10^{-12}
300.0	103.45	0.17	9.66×10^8	5.27×10^{-12}
310.0	73.67	0.17	1.09×10^9	3.49×10^{-12}
320.0	53.77	0.18	1.23×10^9	2.38×10^{-12}

k_{R1} is the rate constant for the process of $\text{HO}_2 + \text{HO}_2 \rightarrow \text{IM1} \rightarrow \text{TS1} \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$, respective; I^{CVT} is the rate constant of canonical variational state to transition state theory and κ^{SCT} is the tunneling coefficients in the $\text{HO}_2 + \text{HO}_2$ reaction.

Table S2 shows that the computed CVT/SCT rate constants for Channel R1 (k_{R1}). It is worth noting that the rate constants of these reactions are increased with the increase in temperature. At 298.15 K, the calculated value of k_{R1} was $5.70 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$, which was in good agreement with experimental reports reported by Thiébaud, *et al.*⁶ ($1.9 \times 10^{-12} \pm 2.0 \times 10^{-13} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ at 298 K), McAdam, *et al.*⁹ ($2.91 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ at 298 K), Kanno, *et al.*⁸ ($2.77 \times 10^{-12} - 1.29 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ at in the temperature range of 250.0-350.0 K), Sehested, *et al.*¹² ($3.5 \times 10^{-12} \pm 1.01 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ at 295 K), Stone and Rowley⁷ ($1.04 \times 10^{-11} - 2.31 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ at in the temperature range of 236-309 K), Maricq and Szente¹⁰ ($4.75 \times 10^{-12} - 1.44 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ at in the temperature range of 210 - 363 K), Dobis and Benson¹¹ ($3.82 \times 10^{-12} - 1.85 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ at in the temperature range of 243-368 K), and theoretical values reported by Zhang, *et al.*¹⁴ ($9.52 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ at 300 K). Zhang, *et al.*¹³ ($4.35 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ at 250 K). This indicates that the calculations for the Reaction (1) without and with $(\text{H}_2\text{O})_n$ ($n = 1-3$) at the CCSD(T)-F12/VTZP//M06-2X/aug-cc-pVTZ level of theory are acceptable.



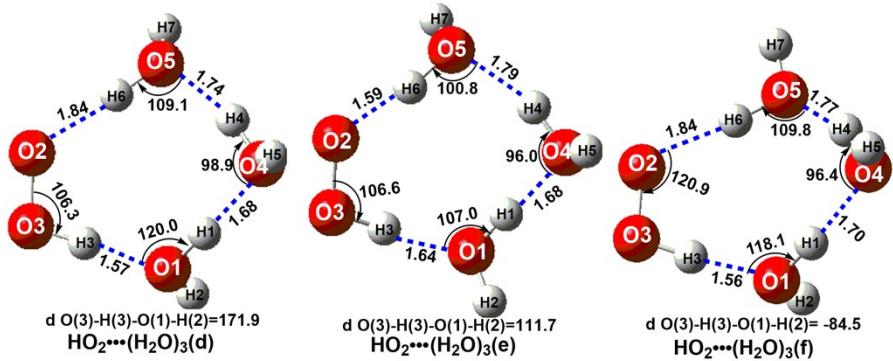


Fig. S2 The optimized geometrical complexes between HO_2 radical and $(\text{H}_2\text{O})_n$ ($n = 1\text{-}3$) at the M06-2X/aug-cc-pVTZ level of theory (bond length Å, bond angle °)

Table S3 Zero point energy (ZPE/(kcal·mol⁻¹)), entropies (S/(cal·mol⁻¹·K⁻¹)), relative energies (ΔE and $\Delta(E + ZPE)/(kcal\cdot mol^{-1})$), enthalpies ($\Delta H(298\text{ K})/(kcal\cdot mol^{-1})$), free energies ($\Delta G(298\text{ K})/(kcal\cdot mol^{-1})$), T_1 diagnostic values and spin contamination $\langle S^2 \rangle$ values for complexes between HO₂ radical and (H₂O)_n ($n = 1-3$)^a

Species	ZPE	S	ΔE	ΔH	ΔG	$\Delta(E + ZPE)$	T_1	$\langle S^2 \rangle$
water molecule								
H ₂ O + HO ₂	22.7	99.7	0.0	0.0	0.0	0.0		
H ₂ O···HO ₂	25.4	70.7(-85±14) ^c	-9.4(-9.14) ^h	-7.6(-7.4±0.9) ^b (-4.76) ^d	1.1	-6.7(-6.73) ^e (-6.37) ^f (-6.10) ^g	0.0249	0.7500
H ₂ O···HO ₂ (a)	25.4	70.7(-85±14) ^c	-9.4	-7.6(-7.4±0.9) ^b (-4.76) ^d	1.1	-6.7(-6.73) ^e (-6.37) ^f (-6.10) ^g	0.0249	0.7500
HO ₂ ···H ₂ O	24.4	78.5	-3.4(-3.54) ^h	-1.9(-2.04) ^h	4.4	-1.7(-1.86) ^e (-2.38) ^h	0.0242	0.7500
HO ₂ ···H ₂ O(a)	24.9	73.1	-3.3(-3.43) ^h	-1.8	6.4	-0.9	0.0242	0.7500
water dimer								
H ₂ O + H ₂ O	27.0	90.2	0.0	0.0	0.0	0.0		
(H ₂ O) ₂	29.3	69.7	-5.2	-3.5	2.9	-3.0	0.0102	0.0000
HO ₂ + (H ₂ O) ₂	38.5	123.3	0.0	0.0	0.0	0.0		
(H ₂ O) ₂ ···HOO	41.1	89.0	-11.3(-11.44) ^h	-9.7	3.0	-8.7	0.0214	0.7500
(H ₂ O) ₂ ···HOO(a)	41.5	81.6	-10.5	-8.9	3.5	-7.4	0.0230	0.7500
(H ₂ O) ₂ ···HOO(b)	41.1	80.9	-11.0	-9.4	3.2	-8.4	0.0225	0.7500
(H ₂ O) ₂ ···HOO(c)	41.9	79.1	-11.3	-9.8	3.4	-7.9	0.0226	0.7500
HO ₂ ···(H ₂ O) ₂	41.5	83.2	-15.6	-13.9	-2.3	-12.9	0.0225	0.7500
HO ₂ ···(H ₂ O) ₂ (a)	41.4	84.1	-15.4(-15.46) ^h	-13.6	-2.0	-12.6	0.0225	0.7500
HO ₂ ···(H ₂ O) ₂ (b)	41.4	84.0	-15.4	-13.7	-1.0	-12.5	0.0225	0.7500
HO ₂ ···(H ₂ O) ₂ (c)	41.5	83.2	-15.8(-15.80) ^h	-14.1	-2.1	-12.9	0.0225	0.7500
water trimer								
(H ₂ O) ₂ + H ₂ O	42.9	113.74	0.0	0.0	0.0	0.0		
(H ₂ O) ₃	46.1	79.72	-11.5	-9.3	1.2	-7.9	0.0104	0.0000
HO ₂ + (H ₂ O) ₃	55.2	134.3	0.0	0.0	0.0	0.0		
(H ₂ O) ₃ ···HOO	56.7	102.6	-11.8	-10.5	-1.1	-10.2	0.0198	0.7500

(H ₂ O) ₃ ···HOO(a)	56.8	101.7	-11.8	-10.5	-0.8	-10.1	0.0201	0.7500
(H ₂ O) ₃ ···HOO(b)	56.5	99.5	-11.1	-10.6	-0.2	-9.9	0.0201	0.7500
(H ₂ O) ₃ ···HOO(c)	56.8	101.7	-11.8	-10.5	-0.8	-10.1	0.0201	0.7500
(H ₂ O) ₃ ···HOO(d)	56.8	102.6	-11.8	-10.5	-1.1	-10.2	0.0198	0.7500
(H ₂ O) ₃ ···HOO(e)	56.6	103.5	-11.3	-10.1	-1.0	-9.9	0.0198	0.7500
(H ₂ O) ₃ ···HOO(f)	56.8	101.7	-11.8	-10.5	-0.8	-10.1	0.0201	0.7500
HO ₂ ···(H ₂ O) ₃	57.2	98.7	-14.5	-13.3	-2.7	-12.7	0.0206	0.7500
HO ₂ ···(H ₂ O) ₃ (a)	56.9	100.6	-14.9	-13.3	-3.2	-12.6	0.0206	0.7500
HO ₂ ···(H ₂ O) ₃ (b)	56.9	100.7	-14.2	-13.3	-3.2	-12.6	0.0206	0.7500
HO ₂ ···(H ₂ O) ₃ (c)	57.1	100.4	-11.8	-10.4	-0.3	-9.9	0.0205	0.7500
HO ₂ ···(H ₂ O) ₃ (d)	57.2	98.6	-14.6	-13.3	-2.7	-12.5	0.0206	0.7500
HO ₂ ···(H ₂ O) ₃ (e)	56.9	92.3	-11.7	-10.9	1.6	-9.5	0.0218	0.7500
HO ₂ ···(H ₂ O) ₃ (f)	56.9	100.6	-14.2	-13.0	-2.9	-12.5	0.0206	0.7500

^a ZPE and S values obtained at M06-2X/aug-cc-pVTZ level of theory; The energy values are obtained at CCSD(T)-F12/VTZP level whereas the H and G corrections are taken from the M06-2X/aug-cc-pVTZ level.

Available Experimental values

^b Value was from Ref.⁸ and was obtained using near-infrared two-tone frequency modulation spectroscopy at 250 - 350 K and 50 Torr with N₂ diluent.

^c Value was from Ref.¹⁵ and was obtained using Fourier transform infrared absorption spectroscopy.

ⁱ Value was from Ref.¹⁶ and was obtained using Laser induced fluorescence.

Available Theoretical values

^d Value was from Ref.¹⁷ and was calculated at the CCSD(T)/6-311++G(2df,2p)

^e Value was from Ref.¹⁴ and was calculated at the UCCSD(T)/aug-cc-pVTZ//UMP2/6-311+g(2df,2p) level of theory.

^f Value was from Ref.³ and was calculated at the CCSD(T)/6-311++G(3d,2p)//B3LYP/6-311G(2d,2p) level of theory.

^g Value was from Ref.¹⁸ and was calculated at the G2M/B3LYP-6-311G(d,p) level of theory.

^h Value was from Ref.¹⁹ and was calculated at the G3//HF/6-31G* level of theory.

Though some isomers shown in Table S3 have positive Gibbs free energy of formation, and thus they would not form spontaneously owing to the large entropic penalty.²⁰ Catalyzed reactions starting from hydrogen bonded complexes between catalyst and reactant remains a major route to estimate the catalytic effect of acidic, neutral and basic catalysts on atmospheric reaction in tropospheric conditions.²¹⁻²⁵

Table S4 Equilibrium constants of complexes between HO₂ radical and (H₂O)_n (*n* = 1-3) ^{a,b,c,d}

T/K	H ₂ O···HO ₂	H ₂ O···HO ₂ (a)	HO ₂ ···H ₂ O	HO ₂ ···H ₂ O(a)	[H ₂ O] ^e	[(H ₂ O) ₂] ^e
275.0	1.00×10 ⁻¹⁸	2.05×10 ⁻¹⁸	1.43×10 ⁻²²	1.86×10 ⁻²³	1.89×10 ¹⁷	1.20×10 ¹⁴
280.0	7.95×10 ⁻¹⁹	8.12×10 ⁻¹⁸	1.36×10 ⁻²²	1.68×10 ⁻²³	2.58×10 ¹⁷	2.04×10 ¹⁴
290.0	5.13×10 ⁻¹⁹	5.65×10 ⁻¹⁹	1.25×10 ⁻²²	1.40×10 ⁻²³	4.78×10 ¹⁷	5.91×10 ¹⁴
298.15	3.67×10 ⁻¹⁹	3.68×10 ⁻¹⁹	1.18×10 ⁻²²	1.22×10 ⁻²³	7.37×10 ¹⁷	1.24×10 ¹⁵
298.15	(8.12×10 ⁷) ^{c,d}	(8.12×10 ⁷) ^{c,d}	(2.70×10 ⁴) ^{c,d}	(2.60×10 ³) ^{c,d}		
300.0	3.41×10 ⁻¹⁹	3.15×10 ⁻¹⁹	1.16×10 ⁻²²	1.18×10 ⁻²³	8.58×10 ¹⁷	1.62×10 ¹⁵
310.0	2.33×10 ⁻¹⁹	2.00×10 ⁻¹⁹	1.08×10 ⁻²²	1.01×10 ⁻²³	1.46×10 ¹⁸	4.06×10 ¹⁵
320.0	1.64×10 ⁻¹⁹	1.10×10 ⁻¹⁹	1.02×10 ⁻²²	8.75×10 ⁻²⁴	2.35×10 ¹⁸	9.24×10 ¹⁵
T/K	(H ₂ O) ₂ ···HOO	(H ₂ O) ₂ ···HOO(a)	(H ₂ O) ₂ ···HOO(b)	(H ₂ O) ₂ ···HOO(c)	HO ₂ ···(H ₂ O) ₂	HO ₂ ···(H ₂ O) ₂ (a)
275.0	3.63×10 ⁻²⁰	3.68×10 ⁻²¹	1.83×10 ⁻²⁰	1.22×10 ⁻²⁰	1.01×10 ⁻¹⁷	6.55×10 ⁻¹⁸
280.0	2.71×10 ⁻²⁰	2.69×10 ⁻²¹	1.29×10 ⁻²⁰	8.54×10 ⁻²¹	6.51×10 ⁻¹⁸	4.27×10 ⁻¹⁸
290.0	1.57×10 ⁻²⁰	1.48×10 ⁻²¹	6.68×10 ⁻²¹	4.34×10 ⁻²¹	2.82×10 ⁻¹⁸	1.90×10 ⁻¹⁸
298.15	1.03×10 ⁻²⁰	9.40×10 ⁻²²	4.03×10 ⁻²¹	2.58×10 ⁻²¹	2.30×10 ⁻¹⁸	1.02×10 ⁻¹⁸
298.15	(3.84×10 ³) ^{c,d}	(3.50×10 ²) ^{c,d}	(1.50×10 ³) ^{c,d}	(9.61×10 ²) ^{c,d}	(8.56×10 ⁵) ^{c,d}	(3.81×10 ⁵) ^{c,d}
300.0	9.42×10 ⁻²¹	8.51×10 ⁻²²	3.61×10 ⁻²¹	2.30×10 ⁻²¹	1.29×10 ⁻¹⁸	8.94×10 ⁻¹⁹
310.0	5.86×10 ⁻²¹	5.06×10 ⁻²²	2.03×10 ⁻²¹	1.27×10 ⁻²¹	6.23×10 ⁻¹⁹	4.42×10 ⁻¹⁹
320.0	3.76×10 ⁻²¹	3.12×10 ⁻²²	1.18×10 ⁻²¹	7.31×10 ⁻²²	3.15×10 ⁻¹⁹	2.28×10 ⁻¹⁹
T/K	HO ₂ ···(H ₂ O) ₂ (b)	HO ₂ ···(H ₂ O) ₂ (c)	[(H ₂ O) ₃] ^e	(H ₂ O) ₃ ···HOO	(H ₂ O) ₃ ···HOO(a)	(H ₂ O) ₃ ···HOO(b)
275.0	7.16×10 ⁻¹⁸	1.01×10 ⁻¹⁷	3.29×10 ¹²	1.55×10 ⁻¹⁸	6.37×10 ⁻¹⁹	2.30×10 ⁻¹⁹
280.0	4.67×10 ⁻¹⁸	6.49×10 ⁻¹⁸	5.85×10 ¹²	9.34×10 ⁻¹⁹	4.60×10 ⁻¹⁹	1.66×10 ⁻¹⁹
290.0	2.08×10 ⁻¹⁸	2.81×10 ⁻¹⁸	1.89×10 ¹³	8.90×10 ⁻¹⁹	2.48×10 ⁻¹⁹	8.94×10 ⁻²⁰
298.15	1.12×10 ⁻¹⁸	1.48×10 ⁻¹⁸	5.15×10 ¹³	6.02×10 ⁻¹⁹	1.55×10 ⁻¹⁹	5.57×10 ⁻²⁰
298.15	(4.16×10 ⁵) ^{c,d}	(5.52×10 ⁵) ^{c,d}		(9.30×10 ³) ^{c,d}	(2.39×10 ³) ^{c,d}	(8.60×10 ²) ^{c,d}
300.0	9.76×10 ⁻¹⁹	1.29×10 ⁻¹⁸	5.82×10 ¹³	3.45×10 ⁻¹⁹	1.40×10 ⁻¹⁹	5.02×10 ⁻²⁰
310.0	4.82×10 ⁻¹⁹	6.22×10 ⁻¹⁹	1.60×10 ¹⁴	1.00×10 ⁻¹⁹	8.17×10 ⁻²⁰	2.93×10 ⁻²⁰
320.0	2.49×10 ⁻¹⁹	3.14×10 ⁻¹⁹	3.91×10 ¹⁴	8.11×10 ⁻²⁰	4.95×10 ⁻²⁰	1.77×10 ⁻²⁰
T/K	(H ₂ O) ₃ ···HOO(c)	(H ₂ O) ₃ ···HOO(d)	(H ₂ O) ₃ ···HOO(e)	(H ₂ O) ₃ ···HOO(f)	HO ₂ ···(H ₂ O) ₃	HO ₂ ···(H ₂ O) ₃ (a)
275.0	6.33×10 ⁻¹⁹	1.02×10 ⁻¹⁸	7.87×10 ⁻¹⁹	6.38×10 ⁻¹⁹	3.47×10 ⁻¹⁷	3.41×10 ⁻¹⁷
280.0	4.57×10 ⁻¹⁹	7.34×10 ⁻¹⁹	5.75×10 ⁻¹⁹	4.61×10 ⁻¹⁹	2.31×10 ⁻¹⁷	2.27×10 ⁻¹⁷
290.0	2.46×10 ⁻¹⁹	3.96×10 ⁻¹⁹	3.18×10 ⁻¹⁹	2.48×10 ⁻¹⁹	1.07×10 ⁻¹⁷	1.05×10 ⁻¹⁷
298.15	1.54×10 ⁻¹⁹	2.47×10 ⁻¹⁹	2.02×10 ⁻¹⁹	1.55×10 ⁻¹⁹	5.93×10 ⁻¹⁸	2.85×10 ⁻¹⁸
298.15	(2.37×10 ³) ^{c,d}	(3.82×10 ³) ^{c,d}	(3.12×10 ³) ^{c,d}	(2.40×10 ³) ^{c,d}	(9.17×10 ⁴) ^{c,d}	(4.41×10 ⁴) ^{c,d}
300.0	1.39×10 ⁻¹⁹	2.23×10 ⁻¹⁹	1.83×10 ⁻¹⁹	1.40×10 ⁻¹⁹	5.14×10 ⁻¹⁸	2.50×10 ⁻¹⁸
310.0	8.11×10 ⁻²⁰	1.30×10 ⁻¹⁹	1.09×10 ⁻¹⁹	8.19×10 ⁻²⁰	2.63×10 ⁻¹⁸	1.27×10 ⁻¹⁸
320.0	4.92×10 ⁻²⁰	7.91×10 ⁻²⁰	6.75×10 ⁻²⁰	4.96×10 ⁻²⁰	1.41×10 ⁻¹⁸	6.74×10 ⁻¹⁹
T/K	HO ₂ ···(H ₂ O) ₃ (b)	HO ₂ ···(H ₂ O) ₃ (c)	HO ₂ ···(H ₂ O) ₃ (d)	HO ₂ ···(H ₂ O) ₃ (e)	HO ₂ ···(H ₂ O) ₃ (f)	
275.0	1.70×10 ⁻¹⁷	2.57×10 ⁻¹⁹	1.62×10 ⁻¹⁷	2.94×10 ⁻²⁰	2.42×10 ⁻²¹	
280.0	1.13×10 ⁻¹⁷	1.86×10 ⁻¹⁹	1.07×10 ⁻¹⁷	2.10×10 ⁻²⁰	2.15×10 ⁻²¹	

290.0	1.02×10^{-17}	1.01×10^{-19}	4.93×10^{-18}	1.11×10^{-20}	1.72×10^{-21}
298.15	5.84×10^{-18}	6.35×10^{-20}	2.72×10^{-18}	6.83×10^{-21}	1.45×10^{-21}
298.15	$(9.03 \times 10^4)^{c,d}$	$(9.81 \times 10^2)^{c,d}$	$(4.42 \times 10^4)^{c,d}$	$(1.05 \times 10^2)^{c,d}$	$(2.25 \times 10^1)^{c,d}$
300.0	5.22×10^{-18}	5.73×10^{-20}	2.38×10^{-18}	6.13×10^{-21}	1.40×10^{-21}
310.0	2.67×10^{-18}	3.38×10^{-20}	1.21×10^{-18}	3.52×10^{-21}	1.16×10^{-21}
320.0	1.43×10^{-18}	2.06×10^{-20}	6.41×10^{-19}	2.09×10^{-21}	9.73×10^{-22}

^a Equilibrium constants in units of $\text{cm}^3 \cdot \text{molecule}^{-1}$;

^b All equilibrium constants were calculated by using energies computed at CCSD(T)-F12/VTZP level and partition functions obtained at M06-2X/aug-cc-pVTZ level.

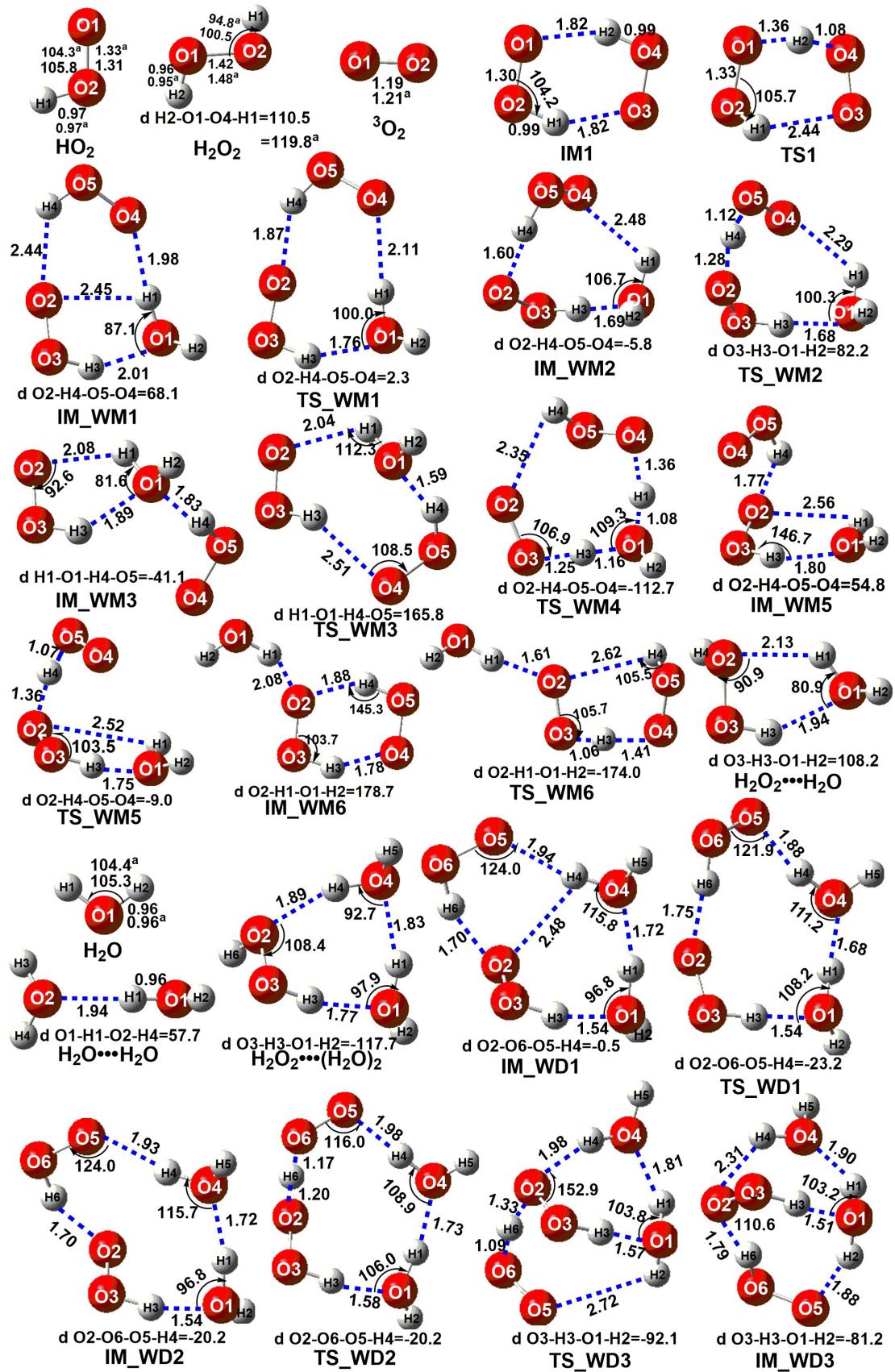
^c The concentration of the corresponding complexes at 298.15 K

^d The concentration have been calculated using 100% relative humidity.

^e Value was from Ref.²⁶

The equilibrium constant of $\text{H}_2\text{O}\cdots\text{HO}_2$ and $\text{HO}_2\cdots\text{H}_2\text{O}$ at 298.15 K is respectively 3.67×10^{-19} and $1.18 \times 10^{-22} \text{ cm}^3 \cdot \text{molecule}^{-1}$. Taking into account typical tropospheric concentrations of $7.37 \times 10^{17} \text{ cm}^3 \cdot \text{molecule}^{-1}$ of H_2O and $3.00 \times 10^8 \text{ cm}^3 \cdot \text{molecule}^{-1}$ of HO_2 , it is estimated that the atmospheric concentration of the $\text{H}_2\text{O}\cdots\text{HO}_2$ and $\text{HO}_2\cdots\text{H}_2\text{O}$ complex is respectively $8.12 \times 10^7 \text{ cm}^3 \cdot \text{molecule}^{-1}$ and $2.70 \times 10^4 \text{ cm}^3 \cdot \text{molecule}^{-1}$, respectively. These results are good agreement with the report of Alongi *et al*¹⁹ that the concentration of $\text{H}_2\text{O}\cdots\text{HO}_2$ and $\text{HO}_2\cdots\text{H}_2\text{O}$ was respectively $6.6 \times 10^7 \text{ cm}^3 \cdot \text{molecule}^{-1}$ and $6.9 \times 10^4 \text{ cm}^3 \cdot \text{molecule}^{-1}$.

For $\text{HO}_2\cdots(\text{H}_2\text{O})_2$ complex, at 298.15 K, our predicted value of equilibrium constant is $2.30 \times 10^{-18} \text{ cm}^3 \cdot \text{molecule}^{-1}$, which is close to the value reported by Alongi *et al*, ¹⁹ meanwhile, for $\text{HO}_2\cdots(\text{H}_2\text{O})_3$ complexes, at 298 K, our predicted equilibrium constant is $5.93 \times 10^{-18} \text{ cm}^3 \cdot \text{molecule}^{-1}$, which is also chose to the reported values in water-assisted $\text{HO}_2 + \text{HS} \rightarrow \text{H}_2\text{O} + {}^3\text{O}_2$ reaction,²⁷ where the equilibrium constant of $\text{HO}_2\cdots(\text{H}_2\text{O})_2$ and $\text{HO}_2\cdots(\text{H}_2\text{O})_3$ complexes at 298.15 K is respectively 8.79×10^{-19} and $4.70 \times 10^{-18} \text{ cm}^3 \cdot \text{molecule}^{-1}$.



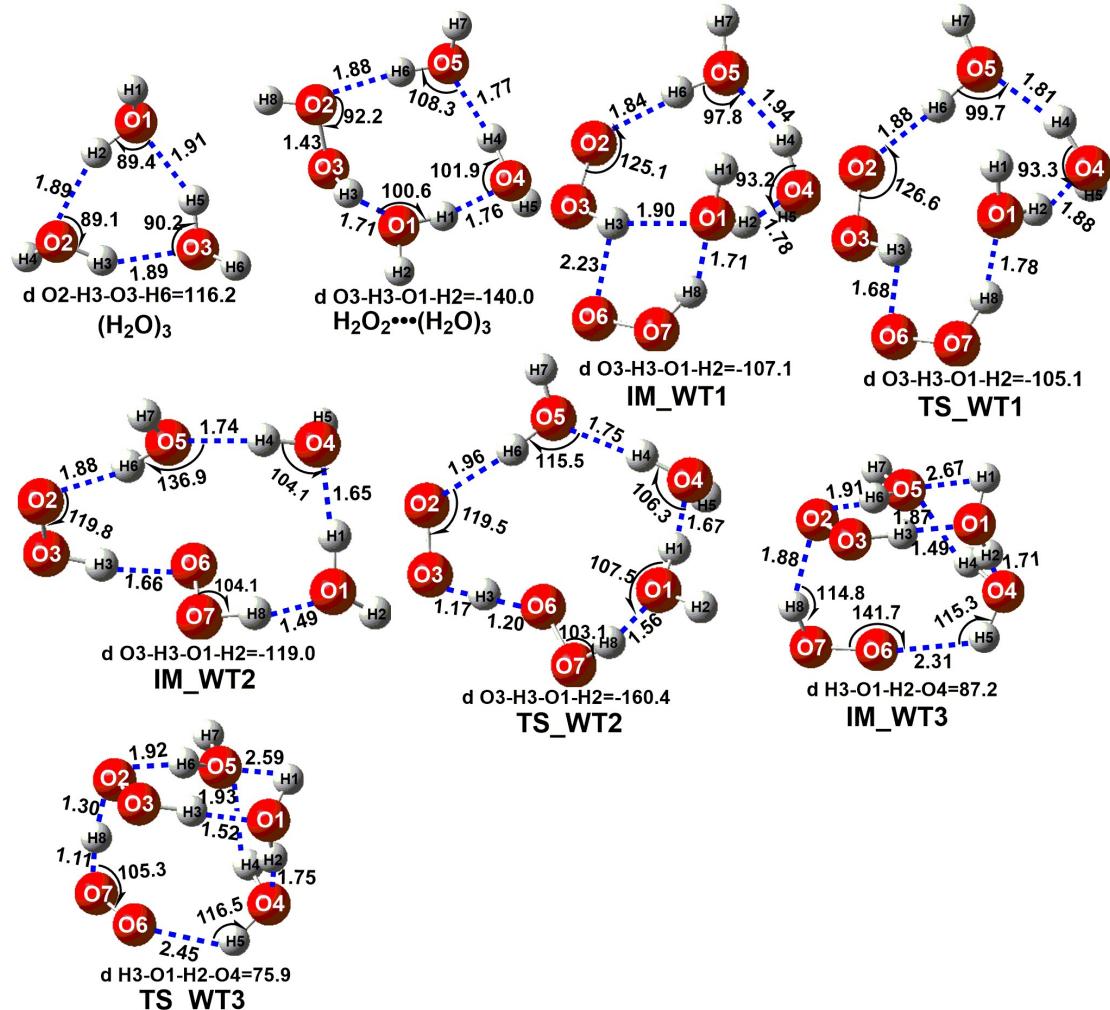


Table S5 Zero point energy (ZPE/(kcal·mol⁻¹)), relative energies (ΔE and $\Delta(E + ZPE)$ /(kcal·mol⁻¹)), enthalpies ($\Delta H(298.15\text{ K})$ /(kcal·mol⁻¹)), free energies ($\Delta G(298.15\text{ K})$ /(kcal·mol⁻¹)), T_1 diagnostic values, and spin contamination $\langle S^2 \rangle$ values for the $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction without and with catalyst $(\text{H}_2\text{O})_n$ ($n = 1-3$)^a

System	<i>S</i>	ZPE	ΔE	ΔH	ΔG	$\Delta(E + ZPE)$	T_1	S^2
No catalysis								
$\text{HO}_2 + \text{HO}_2$	109.2	18.3	0.0	0.0	0.0	0.0		
IM1	74.6	20.9	-11.9	-10.1	0.2	-9.3	0.0313	2.0000
TS1	72.8	17.7	0.4	-1.4	9.5	-0.3	0.0370	2.0001
$\text{H}_2\text{O}_2 + {}^3\text{O}_2$	104.6	19.5	-38.9	-37.7(-37.1 ± 1.4) ^b	-36.4	-37.7		
Water catalysis								
$\text{H}_2\text{O} + \text{HO}_2 + \text{HO}_2$	154.3	31.8	0.0	0.0	0.0	0.0		
$\text{H}_2\text{O}\cdots\text{HO}_2 + \text{HO}_2$	125.3	34.6	-9.4	-7.6	1.1	-6.7		
IM_WM1	98.8	35.8	-16.7	-13.5	3.0	-12.8	0.0273	2.0000
TS_WM1	90.5	36.0	-16.0	-13.4	5.6	-11.9	0.0270	2.0000
IM_WM2	88.8	36.5	-21.7	-18.6	0.7	-17.1	0.0215	2.0000
TS_WM2	88.9	33.0	-9.9	-10.3	9.2	-8.8	0.0324	2.0001
IM_WM3	90.7	36.2	-15.6	-12.8	6.1	-11.3	0.0294	2.0000
TS_WM3	89.1	36.3	-15.5	-12.7	6.8	-11.0	0.0271	2.0000
TS_WM4	90.5	32.9	12.3	8.4	32.1	11.1	0.0277	2.0001
IM_WM5	95.0	35.5	-11.8	-9.0	8.6	-8.1	0.0295	2.0000
TS_WM5	90.1	33.3	-8.9	-9.0	10.1	-7.5	0.0225	2.0001
$\text{HO}_2\cdots\text{H}_2\text{O} + \text{HO}_2$	133.0	33.6	-3.4	-1.9	4.4	-1.7		
IM_WM6	97.9	35.9	-14.8	-11.6	5.2	-10.8	0.0281	2.0000
TS_WM6	102.3	31.8	-3.9	-4.6	10.9	-4.0	0.0231	2.0000
$\text{H}_2\text{O}_2\cdots\text{H}_2\text{O} + {}^3\text{O}_2$	121.1	35.6	-46.3	-43.4	-33.5	-42.5		
$\text{H}_2\text{O}_2 + \text{H}_2\text{O} + {}^3\text{O}_2$	149.6	33.1	-38.7	-37.6	-36.3	-37.5		
Water dimer catalysis								
$(\text{H}_2\text{O})_2 + \text{HO}_2 + \text{HO}_2$	177.9	47.7	0.0	0.0	0.0	0.0		
$\text{HO}_2\cdots(\text{H}_2\text{O})_2 + \text{HO}_2$	137.8	50.7	-15.6	-13.9	-2.3	-12.9		
IM_WD1	104.3	52.1	-24.7	-21.8	-0.2	-20.6	0.0258	2.0000
TS_WD1	103.4	51.7	-23.1	-20.9	1.0	-19.4	0.0255	2.0000
IM_WD2	104.9	52.0	-24.7	-21.9	-0.4	-20.7	0.0258	2.0000
TS_WD2	102.7	48.7	-11.6	-12.3	9.7	-10.9	0.0255	2.0002
IM_WD3	105.3	51.9	-23.2	-20.4	0.9	-19.3	0.0262	2.0000
TS_WD3	99.9	49.4	-15.4	-15.6	7.3	-13.9	0.0295	2.0001
$\text{H}_2\text{O}_2\cdots(\text{H}_2\text{O})_2 + {}^3\text{O}_2$	134.5	51.7	-53.1	-46.0	-53.5	-49.1		
Water trimer catalysis								
$(\text{H}_2\text{O})_3 + \text{HO}_2 + \text{HO}_2$	188.9	66.4	0.0	0.0	0.0	0.0		
$\text{HO}_2\cdots(\text{H}_2\text{O})_3 + \text{HO}_2$	153.3	66.4	-14.5	-13.3	-2.7	-12.7		
IM_WT1	120.3	68.3	-21.4	-18.3	2.2	-17.5	0.0237	2.0000
TS_WT1	115.3	68.0	-20.1	-17.9	4.1	-16.5	0.0241	2.0000
IM_WT2	119.7	67.8	-23.7	-21.3	-0.5	-20.3	0.0240	2.0000
TS_WT2	120.2	64.1	-9.3	-10.6	9.9	-9.6	0.0278	2.0002
IM_WT3	118.2	67.7	-20.1	-17.6	3.6	-18.8	0.0238	2.0000
TS_WT3	112.3	65.2	-13.6	-14.3	8.6	-18.4	0.0235	2.0002
$\text{H}_2\text{O}_2\cdots(\text{H}_2\text{O})_3 + {}^3\text{O}_2$	151.8	67.0	-49.7	-47.4	-36.2	-47.1		

^a ZPE obtained at M06-2X/aug-cc-pVTZ level of theory; The energy values are obtained at CCSD(T)-F12/VTZP level whereas the *H* and *G* corrections are taken from the M06-2X/aug-cc-pVTZ level.

^b Value was from Ref.²⁹

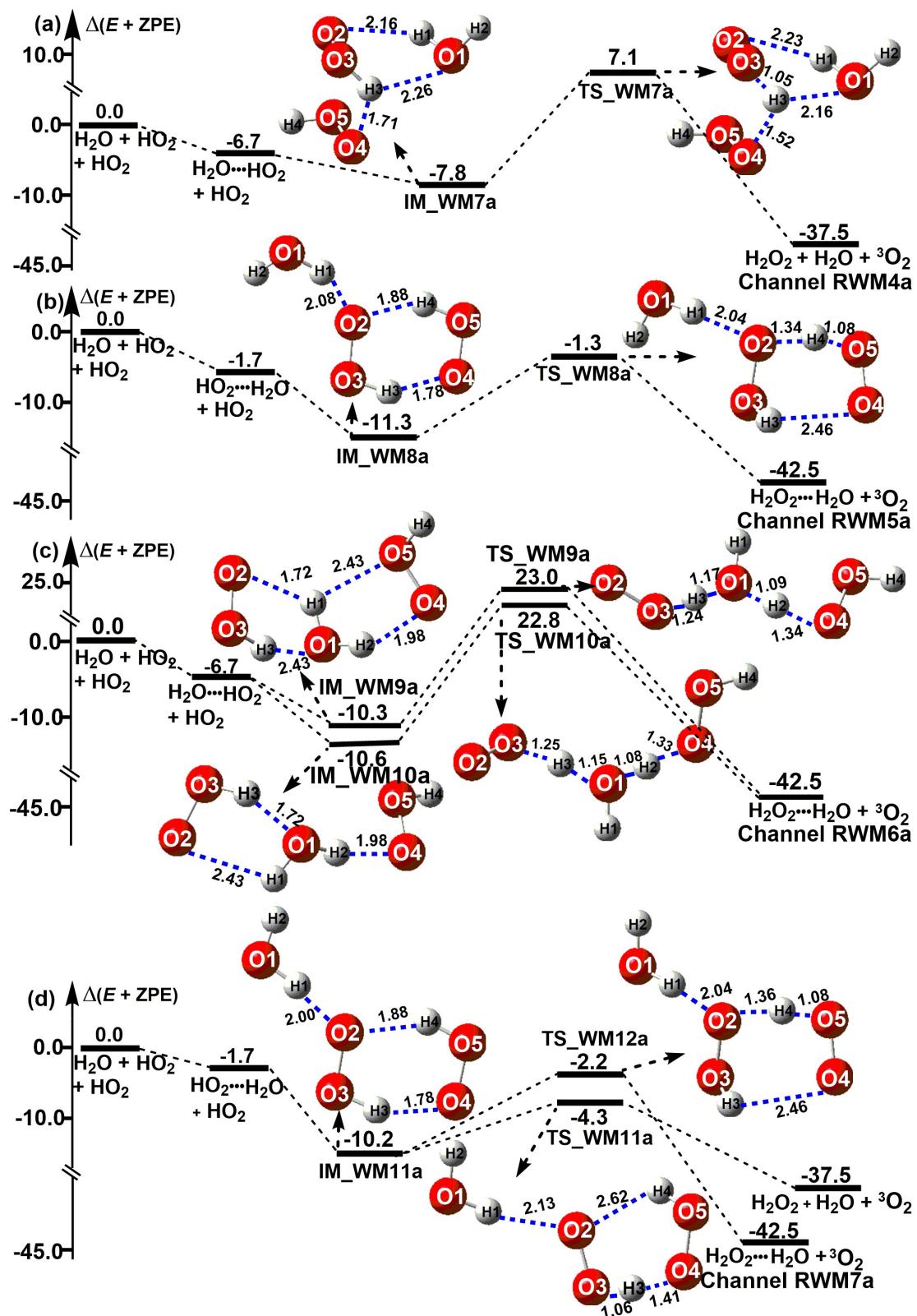


Fig. S4 Schematic energy diagrams for the unfavorable channels in H_2O -assisted $HO_2 + HO_2 \rightarrow H_2O_2 + {}^3O_2$ reaction occurring through one-step process ($\text{kcal}\cdot\text{mol}^{-1}$) at the CCSD(T)-F12/VTZP //M06-2X/aug-cc-pVTZ level

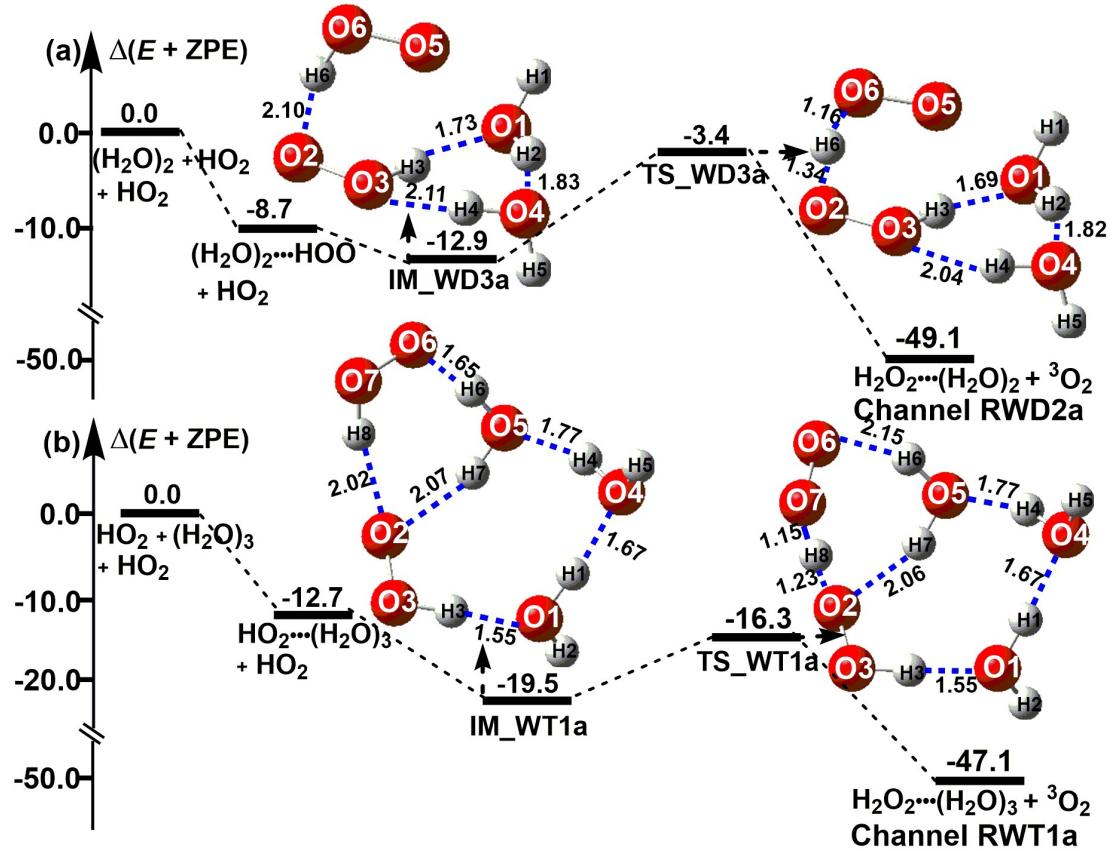


Fig. S5 Schematic energy diagrams for the unfavorable channels in $(\text{H}_2\text{O})_2$ and $(\text{H}_2\text{O})_3$ -assisted $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction occurring through one-step process (kcal·mol⁻¹) at the CCSD(T)-F12/VTZP//M06-2X/aug-cc-pVTZ level

Table S6 The calculated k_{uni} (s^{-1}) for the $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction with $(\text{H}_2\text{O})_n$ ($n = 1\text{-}3$) within the temperature range of 275.0–320.0 K

T/K	$k_{\text{uni}}(\text{RWM1})$	$k_{\text{uni}}(\text{RWM3})$	$k_{\text{uni}}(\text{RWM4})$	$k_{\text{uni}}(\text{RWD1})$	$k_{\text{uni}}(\text{RWD2})$	$k_{\text{uni}}(\text{RWT1})$	$k_{\text{uni}}(\text{RWT2})$
275.0	7.62×10^6	1.17×10^{11}	2.31×10^7	3.16×10^9	3.56×10^7	3.26×10^3	2.34×10^{10}
280.0	9.20×10^6	1.18×10^{11}	2.55×10^7	3.28×10^9	4.15×10^7	4.66×10^3	2.37×10^{10}
290.0	1.32×10^7	1.21×10^{11}	3.08×10^7	3.52×10^9	5.56×10^7	9.17×10^3	2.42×10^{10}
298.15	1.74×10^7	1.22×10^{11}	3.58×10^7	3.70×10^9	6.95×10^7	1.54×10^4	2.46×10^{10}
300.0	1.84×10^7	1.23×10^{11}	3.70×10^7	3.74×10^9	7.29×10^7	1.72×10^4	2.46×10^{10}
310.0	2.53×10^7	1.24×10^{11}	4.40×10^7	3.95×10^9	9.39×10^7	3.10×10^4	2.50×10^{10}
320.0	3.39×10^7	1.26×10^{11}	5.21×10^7	4.15×10^9	1.19×10^8	5.37×10^4	2.53×10^{10}

Table S7 Rate constants and pseudo-first-order rate constants ($\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$) for the unfavorable channels involved in $(\text{H}_2\text{O})_n$ ($n = 1-3$) catalyzed $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction within the temperature range of 275.0–320.0 K

T/K	k_{RWM2}	k_{RWM4a}	k_{RWM5a}	k_{RWM6a}	k_{RWM7a}	k_{RWD2a}	k_{RWT1a}
275.0	2.10×10^{-19}	2.71×10^{-20}	3.00×10^{-15}	3.31×10^{-24}	1.95×10^{-12}	2.51×10^{-19}	2.15×10^{-12}
280.0	2.55×10^{-19}	3.91×10^{-20}	2.60×10^{-15}	3.23×10^{-24}	1.79×10^{-12}	2.44×10^{-19}	1.76×10^{-12}
290.0	3.16×10^{-19}	7.81×10^{-20}	2.03×10^{-15}	3.11×10^{-24}	1.52×10^{-12}	2.35×10^{-19}	1.21×10^{-12}
298.15	4.19×10^{-19}	1.33×10^{-19}	1.69×10^{-15}	3.07×10^{-24}	1.35×10^{-12}	2.30×10^{-19}	7.60×10^{-13}
300.0	4.35×10^{-19}	1.51×10^{-19}	1.63×10^{-15}	3.06×10^{-24}	1.32×10^{-12}	2.29×10^{-19}	6.67×10^{-13}
310.0	5.58×10^{-19}	2.82×10^{-19}	1.35×10^{-15}	3.05×10^{-24}	1.15×10^{-12}	2.27×10^{-19}	3.99×10^{-13}
320.0	6.78×10^{-19}	5.05×10^{-19}	1.14×10^{-15}	3.09×10^{-24}	1.03×10^{-12}	2.28×10^{-19}	2.53×10^{-13}
T/K	k'_{RWM2}	k'_{RWM4a}	k'_{RWM5a}	k'_{RWM6a}	k'_{RWM7a}	k'_{RWD2a}	k'_{RWT1a}
275.0	3.98×10^{-20}	5.14×10^{-21}	8.09×10^{-20}	4.85×10^{-25}	6.86×10^{-18}	1.09×10^{-24}	1.20×10^{-16}
280.0	5.23×10^{-20}	8.01×10^{-21}	9.16×10^{-20}	5.34×10^{-25}	7.75×10^{-18}	1.35×10^{-24}	1.16×10^{-16}
290.0	7.74×10^{-20}	1.91×10^{-20}	1.22×10^{-19}	5.95×10^{-25}	1.02×10^{-17}	2.18×10^{-24}	1.18×10^{-16}
298.15	1.13×10^{-19}	3.60×10^{-20}	1.47×10^{-19}	6.42×10^{-25}	1.21×10^{-17}	2.95×10^{-24}	1.12×10^{-16}
300.0	1.27×10^{-19}	4.41×10^{-20}	1.62×10^{-19}	7.18×10^{-25}	1.33×10^{-17}	3.50×10^{-24}	9.72×10^{-17}
310.0	1.90×10^{-19}	9.60×10^{-20}	2.13×10^{-19}	8.22×10^{-25}	1.70×10^{-17}	5.40×10^{-24}	8.12×10^{-17}
320.0	2.61×10^{-19}	1.94×10^{-19}	2.72×10^{-19}	4.37×10^{-25}	2.11×10^{-17}	7.91×10^{-24}	6.67×10^{-17}
T/K	k'_{RWM3}	k'_{RWM4}	k'_{RWD2}	k'_{RWT1}			
275.0	1.08×10^{-14}	6.51×10^{-17}	6.50×10^{-17}	2.96×10^{-21}			
280.0	1.12×10^{-14}	6.82×10^{-17}	6.66×10^{-17}	3.80×10^{-21}			
290.0	1.23×10^{-14}	7.70×10^{-17}	7.43×10^{-17}	6.65×10^{-21}			
298.15	1.27×10^{-14}	8.20×10^{-17}	7.50×10^{-17}	1.13×10^{-20}			
300.0	1.36×10^{-14}	8.81×10^{-17}	8.37×10^{-17}	1.16×10^{-20}			
310.0	1.48×10^{-14}	9.91×10^{-17}	9.14×10^{-17}	1.87×10^{-20}			
320.0	1.57×10^{-14}	1.09×10^{-16}	9.58×10^{-17}	2.77×10^{-20}			

$k_{\text{RWM2}}, k_{\text{RWM4a}}, k_{\text{RWM5a}}, k_{\text{RWM6a}}$ and k_{RWM7a} is the rate constants for H_2O -assisted the $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction occurring through Channels RWM2, RWM4a, RWM5a, RWM6a and RWM7a, respectively; k_{RWD2a} is the rate constants for $(\text{H}_2\text{O})_2$ -assisted $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction occurring through Channel RWD2a, respectively; k_{RWT1a} is the rate constants for $(\text{H}_2\text{O})_3$ -assisted the $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction occurring through Channels RWT1a. $k'_{\text{RWM2}}, k'_{\text{RWM3}}, k'_{\text{RWM4a}}, k'_{\text{RWM5a}}, k'_{\text{RWM6a}}$ and k'_{RWM7a} is the pseudo-first-order rate constants for Channels RWM2, RWM3, RWM4, RWM4a, RWM5a, RWM6a and RWM7a, respectively; k'_{RWD2} and k'_{RWD2a} is the pseudo-first-order rate constants occurring through the Channels RWD2a and RWD2a; k'_{RWT1} and k'_{RWT1a} is the pseudo-first-order rate constants occurring through the Channels RWT1 and RWT1a.

Table S8 Pseudo-first-order rate constants (k'_t) ($\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$) for $(\text{H}_2\text{O})_n$ ($n = 1\text{-}3$) catalyzed the $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction at various altitudes in troposphere

Altitude	Temp (K)	k_{RWM1}	K_{eq1a}	Concentration ^a	k'_{RWM1}	$k'_{\text{RWM1}}/k_{\text{tot}}$
0 km	298.15	8.96×10^{-11}	3.67×10^{-19}	7.37×10^{17}	2.43×10^{-11}	80.85%
5 km	259.3	4.22×10^{-10}	2.21×10^{-18}	2.41×10^{16}	2.24×10^{-11}	35.05%
10 km	229.7	7.12×10^{-10}	5.90×10^{-18}	4.92×10^{15}	2.07×10^{-11}	6.16%
15 km	212.6	6.25×10^{-9}	4.76×10^{-17}	1.96×10^{13}	5.83×10^{-12}	0.43%
Altitude	Temp (K)	k_{RWD1}	K_{eq1b}	Concentration ^a	k'_{RWD1}	$k'_{\text{RWD1}}/k_{\text{tot}}$
0 km	298.15	1.81×10^{-11}	2.30×10^{-18}	1.24×10^{15}	5.16×10^{-14}	0.17%
5 km	259.3	1.54×10^{-10}	9.52×10^{-17}	2.67×10^{12}	3.91×10^{-14}	0.06%
10 km	229.7	4.81×10^{-10}	3.33×10^{-16}	2.31×10^{11}	3.71×10^{-14}	0.01%
15 km	212.6	1.95×10^{-9}	1.45×10^{-14}	6.26×10^6	1.77×10^{-16}	0.00%
Altitude	Temp (K)	k_{RWT2}	K_{eq1c}	Concentration ^a	k'_{RWT2}	$k'_{\text{RWT2}}/k_{\text{tot}}$
0 km	298.15	3.78×10^{-11}	2.85×10^{-18}	5.15×10^{13}	5.56×10^{-15}	0.02%
5 km	259.3	4.03×10^{-10}	5.39×10^{-16}	2.32×10^{10}	5.03×10^{-15}	0.01%
10 km	229.7	1.81×10^{-9}	8.03×10^{-16}	3.25×10^9	4.71×10^{-15}	0.00%
15 km	212.6	7.06×10^{-9}	1.53×10^{-14}	1.52×10^3	1.64×10^{-19}	0.00%

^aThe Value was from Ref.²⁶

K_{eq1a} , K_{eq1b} and K_{eq1c} is respectively the equilibrium constants for the formation of the bimolecular complexes of $\text{H}_2\text{O}\cdots\text{HO}_2$, $\text{HO}_2\cdots(\text{H}_2\text{O})_2$ and $\text{HO}_2\cdots(\text{H}_2\text{O})_3$.

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**Coordinates and Frequencies of stationary points and the selected points along
the IRC path in the favorable route of $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction
occurring through Channel R1**

Species	Coordinates				Frequencies
HO_2	O	0.05504900	-0.59997400	0.00000000	1256, 1462, 3693
	H	-0.88078400	-0.86566300	0.00000000	
	O	0.05504900	0.70818200	0.00000000	
IM	O	1.46098700	0.56734400	-0.00012700	128, 191, 255, 274, 582, 702, 1297, 1304, 1547, 1563, 3346, 3424
	O	1.24597700	-0.71897100	0.00013200	
	O	-1.46098800	-0.56734300	-0.00012600	
	O	-1.24597500	0.71897000	0.00013100	
	H	0.55517300	0.96457200	-0.00003200	
	H	-0.55517500	-0.96457300	-0.00004100	
$s = -0.43138$	O	1.32587400	0.57622100	-0.17915500	-397, 97, 198, 294, 350, 623, 1209, 1328, 1478, 1560, 2707, 3639
	O	1.16617500	-0.68674900	0.12767000	
	O	-1.27249800	-0.59549900	-0.09614600	
	O	-1.30224500	0.67888300	0.07923600	
	H	0.96247400	1.08496300	0.57033700	
	H	-0.30092300	-0.86779800	-0.02317500	
$s = -1.00617$	O	1.35255200	0.57583600	-0.16661200	-328, 98, 221, 258, 344, 609, 1275, 1316, 1500, 1556, 3103, 3599
	O	1.19470500	-0.68402000	0.12811200	
	O	-1.30353700	-0.59827200	-0.10711000	
	O	-1.29758100	0.68375200	0.08647300	
	H	0.78916800	1.07258900	0.46061400	
	H	-0.35827500	-0.89096600	0.01248500	
$s = -1.67818$	O	1.37982800	0.58053200	-0.14209100	101, 204, 249, 330, 368, 652, 1296, 1310, 1534, 1580, 3242, 3489
	O	1.21644000	-0.68376800	0.12439100	
	O	-1.32904600	-0.59797500	-0.11798600	
	O	-1.29218400	0.68572200	0.09991500	
	H	0.59724700	1.03120000	0.25145600	
	H	-0.39755300	-0.90728700	0.03471100	
$s = -2.25413$	O	-1.39519400	0.58425200	0.11819100	113, 215, 260, 337, 585, 720, 1297, 1308, 1560, 1593, 3235, 3355
	O	-1.23356100	-0.68704600	-0.11887400	
	O	1.35612500	-0.59343300	0.11802300	
	O	1.28185900	0.68866700	-0.11204400	
	H	-0.49961200	0.98199000	-0.03532700	
	H	0.42578700	-0.92151400	-0.00703800	
TS	O	1.31124800	0.58526000	-0.18068200	-1270, 133, 203, 324, 377, 803, 850, 1297, 1455, 1493, 1730, 3696
	O	1.13896700	-0.69424200	0.12452400	
	O	-1.24705400	-0.58773600	-0.09293100	
	O	-1.30765500	0.66678600	0.07711900	
	H	1.03930200	1.08395600	0.60953900	
	H	-0.20334800	-0.84450400	-0.03378400	
$s = 0.4319$	O	1.30501000	0.59757200	-0.17930200	-1387, 165, 193, 357, 411, 658, 1038, 1255, 1456, 1488, 1709, 3748
	O	1.12617300	-0.70061300	0.12137000	
	O	-1.24983200	-0.57925300	-0.09473800	
	O	-1.31314600	0.65272400	0.07813300	
	H	1.05265400	1.08302700	0.61942000	
	H	0.00170600	-0.84647600	-0.02312300	
$s = 1.10306$	O	1.29839900	0.62641000	-0.18111000	-345, -68, 186, 257, 454, 513, 1118, 1429, 146, 169, 3758, 3799
	O	1.13698600	-0.71836400	0.12061200	
	O	-1.27497000	-0.55634800	-0.09661600	
	O	-1.32280800	0.62610400	0.08404400	
	H	1.08630500	1.07712500	0.64533000	
	H	0.21284100	-0.89953600	-0.06076500	
$s = 1.67903$	O	1.28822400	0.64822000	-0.18956100	-231, -60, 189, 213, 355, 470, 1058, 1388, 1462, 1742, 3812, 3824
	O	1.18351600	-0.72230600	0.13180300	
	O	-1.31149500	-0.55810900	-0.09377100	
	O	-1.33949900	0.61762800	0.09071400	
	H	1.12951600	1.07371700	0.66149900	
	H	0.30451400	-0.95718200	-0.17496800	
$s = 2.25508$	O	1.28184600	0.66079100	-0.19682400	-151, -27, 161, 206, 290, 457, 1048, 1365, 1479, 1748, 3837, 3844
	O	1.23261700	-0.71476400	0.14534000	
	O	-1.34864600	-0.56545900	-0.09079700	
	O	-1.36199000	0.60993700	0.09493000	
	H	1.14798700	1.08033600	0.66103400	
	H	0.42139700	-1.00437600	-0.28222700	
H_2O_2	O	0.70227200	0.11402700	-0.05845200	363, 1044, 1355, 3835, 3837
	H	1.01778600	-0.62947300	0.46754300	
	O	-0.70229200	-0.11404000	-0.05842700	
	H	-1.01762100	0.62957800	0.46749100	
O_2	O	0.00000000	0.00000000	0.59492100	1758
	O	0.00000000	0.00000000	-0.59492100	

Coordinates and Frequencies of stationary points and the selected points along the IRC path in the favorable route of $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction with H_2O occurring through Channel RWM1

Species	Coordinates				Frequencies
HO_2	O 0.05504900 H -0.88078400 O 0.05504900	-0.59997400 -0.86566300 0.70818200	0.00000000 0.00000000 0.00000000		1256, 1462, 3693
$\text{H}_2\text{O} \cdots \text{HO}_2$	O -0.97594100 H -0.00384000 O -1.06905300 O 1.61456400 H 1.15596000 H 2.29132100	-0.64074300 -0.81213400 0.66175300 -0.02149300 0.82636400 -0.01037400	0.00819800 -0.00141600 0.01158100 -0.08897000 -0.03582300 0.59076600		165, 191, 218, 248, 342, 499, 642, 1039, 1377, 1532, 1611, 3675, 3814, 3829, 3947
IM_WM1	O -1.73395500 O -2.13740700 H 0.11823600 O 0.85776700 H -1.62992700 H 1.14836400 O 2.05206700 H 2.03217600 O 0.75292200	0.56561300 -0.67038900 1.21852700 1.77991200 -1.15461000 2.30408500 -0.84960500 0.15625200 -1.14106300	-0.05400600 0.13270300 0.19796900 -0.11562700 -0.57599900 0.65974200 0.04869000 0.06032800 -0.05451500		71, 97, 119, 139, 178, 192, 248, 494, 543, 621, 651, 790, 1168, 1243, 1536, 1547, 1633, 3263, 3394, 3594, 3690
TS_WM1	O 0.53135700 O 1.82725200 H 0.29903300 O 1.22780100 H 2.01326600 H 1.30940600 O -2.14046800 H -1.33609600 O -1.73164200	-1.03717000 -1.00513300 1.26494800 1.53953300 -0.02760700 2.36537100 -0.52434200 -1.08334200 0.71219100	-0.00117300 0.02119000 -0.02372500 -0.07889400 0.02502400 0.40057200 -0.01077800 -0.03324000 0.02357600		-36, 32, 95, 163, 188, 231, 255, 282, 387, 419, 569, 672, 1289, 1326, 1477, 1564, 1617, 3327, 3591, 3722, 3952
IM_WM2	O -0.99231400 O -0.46328300 O 1.42212100 O 1.59920400 H -1.14096900 H 0.83688300 H -0.41259600 O -1.28311700 H -1.54420900	-1.00490100 -1.45119000 0.45796400 0.07930300 -0.03296300 -0.54232500 1.95639100 1.53898600 1.65760400	0.63032800 -0.50612600 0.70955200 -0.53278600 0.46597300 -0.72313500 -0.02956300 -0.13352200 -1.05284000		80, 112, 149, 171, 240, 169, 297, 339, 384, 462, 660, 768, 1197, 1259, 1546, 1563, 1623, 3069, 3237, 3757, 3895
$s = -0.39588$	O 0.45978000 O -0.15231000 O -0.97179800 O -1.65150700 H 1.10700000 H -1.14188600 H 1.17598100 O 1.89913400 H 2.19251600	1.18349800 1.44214300 -1.10251600 -0.44945900 0.45417200 0.42056900 -1.52119900 -0.88435300 -0.86805000	0.66098400 -0.46799000 0.50522300 -0.36902900 0.43414100 -0.53497900 -0.11930000 -0.16651600 -1.08123900		-83, 32, 109, 159, 194, 254, 280, 298, 359, 400, 569, 849, 1227, 1341, 1575, 1614, 2505, 3174, 3818, 3933
$s = -0.83633$	O 0.53726800 O -0.05764500 O -1.02087100 O -1.70203200 H 1.10804000 H -1.16227100 H 1.09556400 O 1.84612100 H 2.13593400	1.17133500 1.47177300 -1.05910500 -0.39017100 0.37774500 0.43688300 -0.55550500 -0.97734600 -0.96491500	0.65670300 -0.46529700 0.50838500 -0.36362300 0.43688300 -0.12582700 -0.16987800 -1.08587000		-81, 50, 116, 159, 194, 235, 255, 285, 330, 394, 527, 816, 1275, 1328, 1557, 1584, 1614, 2859, 3122, 3820, 3933
$s = -1.27677$	O 0.63246300 O 0.04939800 O -1.08126000 O -1.75106700 H 1.11807500 H -1.17216500 H 0.99555200 O 1.77493400 H 2.06278800	1.15468300 1.49238000 -1.00710800 -0.31044300 0.30450300 0.43886800 -0.57206400 -1.65303300 -0.13532500 -1.08587600 -0.17250500 -1.07339600	0.65120000 -0.46421000 0.50996200 -0.35474000 0.43886800 -0.12582700 -0.16987800 -0.13532500 -0.17250500 -0.108913200 -0.08587000		-76, 49, 114, 153, 185, 228, 248, 286, 304, 377, 491, 825, 1292, 1323, 1552, 1585, 1613, 3058, 3157, 3825, 3934
$s = -2.02486$	O 0.82300400 O 0.24451500 O -1.19945700 O -1.81646200	1.10774800 1.49836200 -0.90372500 -0.13292400	0.63703300 -0.46223700 0.50946500 -0.33602100		-59, 47, 106, 143, 182, 199, 228, 279, 302, 396, 486, 799, 1298, 1319, 1529, 1593, 1615, 3157, 3268, 3821, 3932

	H	1.15164500	0.18244400	0.43982900	
	H	-1.15701400	0.56698000	-0.58033500	
	H	0.77026600	-1.74779100	-0.14594100	
	O	1.61509700	-1.28340600	-0.17582000	
	H	1.90153300	-1.29007400	-1.09291500	
TS_WM2	O	0.42478200	1.18764500	0.66886100	-1736, 69, 93, 132, 178, 203, 273, 307, 365, 398, 694, 840, 893, 1277, 1459, 1569, 1612, 1682, 3247, 3827, 3938
	O	-0.20815300	1.42051600	-0.47708300	
	O	-0.95235200	-1.12100300	0.49773900	
	O	-1.62058400	-0.48320500	-0.36490100	
	H	1.11000800	0.50522600	0.43356200	
	H	-1.07648600	0.47895900	-0.52467900	
	H	1.22048200	-1.49719400	-0.11875000	
	O	1.92231600	-0.83812000	-0.16370200	
	H	2.21791500	-0.81365500	-1.07745100	
s = 0.35235	O	0.42109900	1.18501300	0.67521800	-1217, -149, 102, 142, 160, 257, 267, 288, 337, 405, 706, 872, 981, 1292, 1564, 1573, 1612, 1680, 3412, 3847, 3949
	O	-0.22108500	1.41463400	-0.48242500	
	O	-0.95477300	-1.12209500	0.49133400	
	O	-1.61687900	-0.49732700	-0.36035300	
	H	1.10663600	0.52045800	0.43778200	
	H	-0.97851400	0.61295700	-0.53094400	
	H	1.22901200	-1.49715800	-0.12042900	
	O	1.92443300	-0.83391000	-0.16257300	
	H	2.22050500	-0.80677500	-1.07602100	
s = 1.10043	O	0.44895600	1.16825900	0.70425900	-366, -144, 33, 102, 127, 147, 237, 241, 291, 295, 462, 801, 1103, 1416, 1533, 1615, 1707, 3577, 3764, 3860, 3959
	O	-0.18448900	1.44288300	-0.50744500	
	O	-0.99504300	-1.09704800	0.47320300	
	O	-1.63232600	-0.50432200	-0.34460900	
	H	1.13288400	0.52621700	0.44195400	
	H	-0.92498700	0.83758100	-0.54012000	
	H	1.21727000	-1.54676800	-0.13088600	
	O	1.90887100	-0.88098800	-0.16241600	
	H	2.20708400	-0.84729900	-1.07489100	
s = 1.49683	O	0.46421800	1.15849200	0.71847900	-353, -115, -30, 106, 120, 167, 209, 234, 279, 298, 430, 788, 1068, 1402, 1530, 1617, 1733, 3593, 3842, 3861, 3960
	O	-0.14064900	1.46984700	-0.51631000	
	O	-1.01678400	-1.08706600	0.46908300	
	O	-1.65442700	-0.49885800	-0.34681500	
	H	1.14127900	0.51260900	0.44822900	
	H	-0.94685700	0.95333500	-0.51559600	
	H	1.20638600	-1.58431700	-0.14046400	
	O	1.89780100	-0.91811700	-0.16402300	
	H	2.19792000	-0.87601800	-1.07548300	
s = 1.93729	O	0.47812800	1.15220100	0.72875300	-143, -89, -12, 104, 121, 181, 195, 229, 274, 297, 422, 791, 1055, 1393, 1535, 1618, 1741, 3599, 3861, 3867
	O	-0.08993000	1.49416200	-0.52357400	
	O	-1.04047100	-1.07728500	0.46523800	
	O	-1.67834500	-0.49192500	-0.35156200	
	H	1.13510600	0.48463300	0.46115300	
	H	-0.96323400	1.10067100	-0.47932600	
	H	1.19434500	-1.62486300	-0.15008700	
	O	1.88641100	-0.95904100	-0.16356200	
	H	2.18744700	-0.90533200	-1.07409000	
O ₂	O	0.00000000	0.00000000	0.59492100	1758
	O	0.00000000	0.00000000	-0.59492100	
H ₂ O ₂ ••H ₂ O	O	0.99438800	-0.66572500	0.11005000	165, 191, 218, 248, 342, 499, 642, 1039, 1377, 1532, 1611, 3675, 3814, 3829, 3947
	H	1.43356700	-0.90682700	-0.71321700	
	O	0.96504400	0.75583900	0.01601800	
	H	0.01210600	0.90672300	-0.10923800	
	O	-1.70188500	-0.00803600	-0.11395500	
	H	-1.13845400	-0.74375300	0.15534400	
	H	-2.36759400	0.08723600	0.57020500	

**Coordinates and Frequencies of stationary points and the selected points along
the IRC path in the favorable route of $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction with
 H_2O occurring through Channel RWM3**

Species	Coordinates				Frequencies
IM_WM5	O	0.36519600	1.19169100	0.67952000	
	O	0.60660900	1.19047600	-0.62448800	
	H	1.05600000	0.32277600	-0.77542400	
	O	1.77276500	-1.15118100	-0.02937400	25, 48, 134, 175, 201, 221,
	H	1.85850400	-0.87922100	0.89297600	288, 302, 358, 401, 460, 580,
	H	2.57494900	-1.63748700	-0.25860900	1209, 1271, 1519, 1542, 1619,
	O	-1.63138000	-0.51057900	0.59265000	3405, 3419, 3790, 3891
	H	-0.73607400	-0.18608900	0.84130700	
$s = -0.39878$	O	-1.70736400	-0.42290500	-0.70583900	
	O	-0.17629500	1.24508900	-0.52550700	
	O	-0.42426000	1.03813800	0.74604200	
	H	-1.01381800	0.23981700	0.74454000	-54, -30, 89, 118, 133, 237,
	O	-1.93504700	-0.95295400	-0.13639300	247, 289, 307, 415, 587, 678,
	H	-1.80393700	-0.62852400	-1.03281300	1194, 1325, 1558, 1585, 1607,
	H	-2.86664900	-1.16708000	-0.05162400	2594, 3313, 3852, 3959
	O	1.71528000	-0.33096900	-0.54252600	
$s = -0.99756$	H	1.04041000	0.41005300	-0.70722600	
	O	1.40082200	-0.85608800	0.58927400	
	O	-0.24448900	1.26573100	-0.52579000	
	O	-0.47878200	1.04438600	0.73917400	
	H	-1.01979200	0.21165400	0.73886400	-67, 31, 79, 107, 151, 208,
	O	-1.90494900	-1.00513100	-0.14046600	242, 256, 290, 402, 462, 606,
	H	-1.77800700	-0.69347000	-1.04182300	1257, 1309, 1533, 1569, 1606,
	H	-2.83012100	-1.24559300	-0.05635200	3092, 3309, 3853, 3958
$s = -1.44706$	O	1.77069100	-0.31186600	-0.53711400	
	H	1.11428800	0.41222600	-0.72131900	
	O	1.42173400	-0.82872300	0.59927500	
	O	-0.29658400	1.27854300	-0.52730900	
	O	-0.52651600	1.05010700	0.73569500	
	H	-1.03005400	0.19433600	0.73557800	-58, 32, 79, 96, 160, 195, 234,
	O	-1.87778500	-0.10495600	-0.14378500	239, 287, 394, 444, 620, 1269,
	H	-1.75456000	-0.73640600	-1.04513600	1306, 1530, 1574, 1605, 3257,
$s = -2.24621$	H	-2.79793800	-1.30978100	-0.06275500	3332, 3853, 3958
	O	1.81160400	-0.28952100	-0.52951400	
	H	1.15623900	0.42576700	-0.72420700	
	O	1.44264300	-0.81131300	0.60197800	
	O	-0.37916300	1.29321600	-0.53023400	
	O	-0.62003300	1.06225900	0.72933600	
	H	-1.06183100	0.17315100	0.72897700	-37, 42, 91, 111, 143, 178,
	O	-1.82199100	-1.12818500	-0.15057800	214, 236, 277, 389, 414, 595,
TS_WM5	H	-1.69534900	-0.81110100	-1.05019400	1272, 1306, 1522, 1578, 1605,
	H	-2.73307700	-1.42245100	-0.08537700	3343, 3424, 3852, 3959
	O	1.87884700	-0.23538800	-0.50780800	
	H	1.21839900	0.46621500	-0.70895300	
	O	1.47632300	-0.79262900	0.59872700	
	O	-0.13645300	-1.23084900	0.53178200	
	O	-0.40057400	-1.03588200	-0.75416400	
	H	-1.01659900	-0.26180900	-0.74811700	-1128, 53, 72, 145, 159, 192,
$s = 0.44935$	O	-1.94825900	0.92905900	0.13346800	260, 305, 369, 419, 721, 791,
	H	-1.81487000	0.59012400	1.02436600	882, 1310, 1512, 1563, 1607,
	H	-2.88335200	1.12775900	0.04967000	1720, 3370, 3850, 3960
	O	1.68467100	0.33967300	0.53867100	
	H	0.96103600	-0.43904700	0.69342400	
	O	1.39483900	0.87087100	-0.57717500	
	O	-0.12125500	1.22426600	-0.54011300	
	O	-0.39510800	1.03196900	0.76404200	
$s = 1.09772$	H	-1.01377000	0.27343300	0.75317500	-1371, -129, -17, 161, 171,
	O	-1.94924500	-0.92670900	-0.13159300	256, 258, 284, 358, 401, 658,
	H	-1.81684000	-0.57961000	-1.01947700	733, 1050, 1262, 1488, 1573,
	H	-2.88466200	-1.12204400	-0.04699900	1607, 1709, 3518, 3850, 3962
	O	1.68197500	-0.35035000	-0.53125700	
	H	0.79747200	0.57108400	-0.69068400	
	O	1.39835800	-0.87203400	0.56441900	
	O	-0.13823300	1.23185200	-0.56086200	-239, -143, -14, 93, 165, 202,

	O	-0.40164500	1.02395800	0.78837800	241, 255, 280, 354, 465, 688, 1117, 1454, 1556, 1605, 1691, 3610, 3700, 3851, 3962
	H	-1.02727900	0.27922900	0.75887500	
	O	-1.94122800	-0.94828700	-0.13030900	
	H	-1.81496900	-0.57510700	-1.00859100	
	H	-2.87587400	-1.14750800	-0.04690000	
	O	1.69614900	-0.36314400	-0.51239000	
	H	0.67332500	0.74429600	-0.72015200	
	O	1.41555700	-0.85699100	0.54227900	
s = 1.64706	O	-0.19752900	1.25634900	-0.56661700	
	O	-0.41257100	1.01242200	0.80981300	
	H	-1.03619400	0.26599800	0.76914500	
	O	-1.92703900	-0.98884600	-0.13572300	-150, -95, -14, 67, 186, 190,
	H	-1.80821300	-0.56118200	-0.99041300	221, 259, 276, 385, 410, 675,
	H	-2.86014500	-1.19804400	-0.05916800	1056, 1409, 1546, 1606, 1736,
	O	1.72847700	-0.35856600	-0.51468500	3611, 3806, 3845, 3959
	H	0.67413100	0.88569300	-0.72449500	
	O	1.43746500	-0.84541700	0.53282800	
s = 2.1965	O	-0.26420100	1.27380000	-0.56583900	
	O	-0.42514300	1.00799600	0.81998600	
	H	-1.01891500	0.23728700	0.78694000	
	O	-1.91002000	-1.03404500	-0.13819700	-97, -59, 53, 67, 170, 192,
	H	-1.79653000	-0.55135700	-0.96424700	226, 246, 269, 368, 418, 659,
	H	-2.84196400	-1.25171500	-0.07185800	1045, 1392, 1549, 1605, 1743,
	O	1.76153600	-0.34883800	-0.52043600	3632, 3835, 3840, 3954
	H	0.65507600	1.03842000	-0.71983200	
	O	1.46311900	-0.83299200	0.52561000	
O ₂	O	0.00000000	0.00000000	0.59492100	1758
H ₂ O ₂ •••H ₂ O	O	0.00000000	0.00000000	-0.59492100	
	O	-0.96509100	0.75582300	-0.01604400	
	O	-0.99438700	-0.66574300	-0.11002200	
	H	-0.01215500	0.90675700	0.10914800	165, 191, 218, 248, 342, 499,
	O	1.70180200	-0.00798700	0.11391300	642, 1039, 1377, 1532, 1611,
	H	2.36828400	0.08709300	-0.56951600	3675, 3814, 3829, 3947
	H	1.13862600	-0.74375100	-0.15577500	
	H	-1.43334200	-0.90684500	0.71336400	

**Coordinates and Frequencies of stationary points and the selected points along
the IRC path in the favorable route of $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction with
 H_2O occurring through Channel RWM4**

Species	Coordinates				Frequencies
IM_WM6	O	0.44692200	0.02984300	-0.01932200	
	O	0.06028300	1.27381800	0.00329100	
	O	-2.41114200	0.22333400	0.01161800	
	H	-0.92995600	1.21226200	0.01269400	
	O	3.42749400	-0.51850100	0.02285400	
	H	2.51842200	-0.20401600	-0.00837600	
	H	3.97318700	0.25994300	-0.09981500	
	O	-2.08178900	-1.03728100	-0.00474300	
	H	-1.09580100	-1.03789100	-0.01407800	
$s = -0.22779$	O	-0.49566300	-0.08498300	-0.11981700	
	O	0.02752300	1.09280200	-0.08807100	
	O	2.34832000	0.32845000	0.22043600	
	H	1.01594300	0.95871800	0.05545700	
	O	-3.54832400	-0.37374700	0.15295200	
	H	-2.62306000	-0.17415500	-0.02643900	
	H	-4.04932600	0.17404200	-0.45360700	
	O	2.16743700	-0.91319600	-0.17877900	
	H	1.66209900	-1.35321300	0.53082000	
$s = -0.59938$	O	-0.48961500	-0.09159300	-0.11612400	
	O	0.00476400	1.10501800	-0.09325100	
	O	2.36507800	0.31799800	0.21979600	
	H	0.98090300	0.99384100	0.08278800	
	O	-3.54474800	-0.37911100	0.15276200	
	H	-2.61898100	-0.17917600	-0.02422300	
	H	-4.04450600	0.16745800	-0.45590100	
	O	2.17848700	-0.91028500	-0.17279400	
	H	1.57084700	-1.31832800	0.47422800	
$s = -0.94241$	O	-0.48460400	-0.09636700	-0.11161700	
	O	-0.01246800	1.11317700	-0.10021700	
	O	2.37742900	0.31516300	0.21928700	
	H	0.95676900	1.01631200	0.10210700	
	O	-3.54155700	-0.38238500	0.15364000	
	H	-2.61548400	-0.18476600	-0.02411700	
	H	-4.04027100	0.16130800	-0.45845800	
	O	2.18964700	-0.91471500	-0.16308300	
	H	1.47140700	-1.27183400	0.39638900	
$s = -1.29974$	O	0.47980000	-0.10047300	0.10631400	
	O	0.02668600	1.11915300	0.10676500	
	O	-2.38684000	0.31361100	-0.21842000	
	H	-0.93938100	1.03398600	-0.11118600	
	O	3.53866100	-0.38484900	-0.15508700	
	H	2.61239300	-0.19056100	0.02461500	
	H	4.03663500	0.15548900	0.46059800	
	O	-2.20009800	-0.92043200	0.14980600	
	H	-1.37532100	-1.21499400	-0.28905400	
TS_WM6	O	0.49883200	0.08445700	-0.12046500	
	O	-0.03271200	-1.09093000	-0.09090900	
	O	-2.34359800	-0.34399200	0.22230200	
	H	-1.07356800	-0.93263700	0.05050900	
	O	3.55002500	0.37050200	0.15490900	
	H	2.62346400	0.17158800	-0.02792000	
	H	4.05184400	-0.17733500	-0.45504600	
	O	-2.16241000	0.92662400	-0.18031400	
	H	-1.68283600	1.36510400	0.54828600	
$s = 0.53351$	O	-0.49761000	-0.07199600	-0.12162900	
	O	0.03422200	1.07645200	-0.09340400	
	O	2.32441200	0.35963300	0.22140100	
	H	1.28869500	0.84662100	0.06752000	
	O	-3.55383600	-0.36523800	0.15616400	
	H	-2.62977700	-0.16834300	-0.02928700	
	H	-4.05640500	0.18059000	-0.45539200	
	O	2.15249300	-0.93425200	-0.18154600	
	H	1.72004000	-1.37566600	0.56926200	

	O	-0.49367700	-0.05277700	-0.12161100	
	O	0.00091800	1.06076200	-0.09972100	
	O	2.33792800	0.37876700	0.22930100	
	H	1.49390600	0.81816200	0.04449100	
s = 1.18504	O	-3.55753500	-0.36696900	0.16093400	-163, -75, -60, 58, 98, 146, 169,
	H	-2.63639800	-0.17325200	-0.03216200	187, 206, 306, 457, 525, 1066,
	H	-4.06342900	0.17460200	-0.45200800	1426, 1465, 1569, 1621, 3585,
	O	2.14231000	-0.94960000	-0.18815600	3752, 3850, 3949
	H	1.76637100	-1.38097900	0.59369700	
	O	-0.50467600	-0.05196700	-0.12136800	
	O	-0.05665300	1.07067200	-0.10074700	
	O	2.40096800	0.37850700	0.25115600	
	H	1.64137400	0.87208300	-0.08733700	-68, -43, 64, 100, 124, 150, 172,
s = 2.0159	O	-3.56513900	-0.37185200	0.16970400	185, 193, 276, 376, 496, 998,
	H	-2.64676100	-0.19536800	-0.05090000	1368, 1459, 1619, 1634, 3739,
	H	-4.07985100	0.16389000	-0.44095500	3774, 3848, 3948
	O	2.12742800	-0.95622200	-0.20384500	
	H	1.86980900	-1.39370300	0.61998600	
	O	-0.51950100	-0.05039100	-0.12069400	
	O	-0.10539300	1.08351500	-0.10021300	
	O	2.45953500	0.36767500	0.26579400	
	H	1.78117800	0.90482100	-0.16531900	-37, 43, 92, 147, 163, 178, 186,
s = 2.72657	O	-3.57648200	-0.37524300	0.17756600	200, 226, 251, 308, 439, 985,
	H	-2.66310800	-0.23508400	-0.08659500	1337, 1473, 1622, 1646, 3795,
	H	-4.10090000	0.15035400	-0.43362400	3822, 3848, 3946
	O	2.12456400	-0.95280500	-0.21376800	
	H	1.92104300	-1.40210700	0.61605100	
O ₂	O	0.00000000	0.00000000	0.59492100	1758
	O	0.00000000	0.00000000	-0.59492100	
	O	-0.96509100	0.75582300	-0.01604400	
	O	-0.99438700	-0.66574300	-0.11002200	
	H	-0.01215500	0.90675700	0.10914800	
H ₂ O ₂ ••H ₂ O	O	1.70180200	-0.00798700	0.11391300	165, 191, 218, 248, 342, 499,
	H	2.36828400	0.08709300	-0.56951600	642, 1039, 1377, 1532, 1611,
	H	1.13862600	-0.74375100	-0.15577500	3675, 3814, 3829, 3947
	H	-1.43334200	-0.90684500	0.71336400	

**Coordinates and Frequencies of stationary points and the selected points along
the IRC path in the favorable route of $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction with
 $(\text{H}_2\text{O})_2$ occurring through Channel RWD1**

Species	Coordinates			Frequencies
IM_WD1	O	-0.63998800	1.82403900	0.10091400
	H	0.22283100	1.37667000	0.10550500
	H	-0.52114300	2.62318800	-0.41626400
	O	-0.60736400	-1.46474000	-0.48760200
	H	-1.52584800	-1.02340000	-0.39443700
	O	-2.62039800	0.02108000	-0.09346400
	H	-3.08625200	-0.08692000	0.73889400
	H	-2.01917100	0.79254600	0.01525600
	O	0.00190600	-1.11427600	0.60805100
	O	2.46697700	-0.41964900	-0.01409800
	H	1.65309800	-0.93016300	0.24469900
	O	2.05842800	0.80955500	-0.15050800
TS_WD1	O	0.06772500	2.05734800	0.38195500
	H	0.79610900	1.41368400	0.40686600
	H	0.42377700	2.83702100	-0.04980900
	O	-1.55424900	-1.59628300	0.04346900
	H	-1.86050100	-0.65597500	-0.20847400
	O	-2.13344700	0.83298200	-0.48263700
	H	-2.90041500	1.19884700	-0.03680200
	H	-1.35015300	1.35129200	-0.18019600
	O	-0.35435400	-1.44165100	0.51555400
	O	2.13299000	-0.84917000	-0.42913700
	H	1.20553900	-1.09417800	-0.20067100
	O	2.30203900	0.36543700	0.00443100
IM_WD2	O	-0.64032000	1.82425500	0.10131700
	H	0.22246200	1.37680100	0.10581600
	H	-0.52171500	2.62278000	-0.41687100
	O	-0.60677900	-1.46462500	-0.48767000
	H	-1.52540300	-1.02351800	-0.39473900
	O	-2.62017700	0.02073700	-0.09377400
	H	-3.08613600	-0.08776800	0.73846000
	H	-2.01916000	0.79232300	0.01537200
	O	0.00191900	-1.11444700	0.60839600
	O	2.46683400	-0.41944300	-0.01416700
	H	1.65309500	-0.93000700	0.24495500
	O	2.05813100	0.80969700	-0.15072600
s = -0.30051	O	-0.44664200	2.07479600	0.38322700
	H	0.39854700	1.59613900	0.41929600
	H	-0.25978200	2.88860500	-0.09048800
	O	-0.79975000	-1.80777000	-0.07287000
	H	-1.45155800	-1.05337200	-0.29657900
	O	-2.26198200	0.27653500	-0.48928500
	H	-3.07336400	0.33976800	0.01974500
	H	-1.67340600	1.00334700	-0.17975600
	O	0.05493300	-1.23668500	0.75676100
	O	1.99405800	-0.52061600	-0.40485100
	H	1.18379200	-0.90154000	0.09913100
	O	2.06885400	0.72962200	-0.16940000
s = -0.85837	O	-0.42594800	2.07563000	0.38325600
	H	0.41407900	1.58709200	0.41182300
	H	-0.23387600	2.89032400	-0.08681100
	O	-0.82211100	-1.79091900	-0.08087500
	H	-1.49465700	-1.04425400	-0.27874900
	O	-2.25262300	0.29702900	-0.49870300
	H	-3.06984500	0.38587300	-0.00305800
	H	-1.65214200	1.01566100	-0.19041800
	O	-0.00244100	-1.24712200	0.76902500
	O	2.02711000	-0.54513600	-0.41748200
	H	1.27791900	-0.93477800	0.11678200
	O	2.07082900	0.72303000	-0.15141600
s = -1.37385	O	-0.40868800	2.07355900	0.38047000
	H	0.42404900	1.57365400	0.41354300
	H	-0.20573100	2.88590500	-0.08894500
	O	-0.84725500	-1.77763100	-0.09325600

	H	-1.52868300	-1.03585700	-0.27669000	1642, 1673, 2768, 3182, 3363, 3684, 3923, 3929
	O	-2.24558600	0.31250200	-0.50439300	
	H	-3.06968500	0.43633300	-0.02830900	
	H	-1.63084500	1.01987100	-0.19738800	
	O	-0.05117800	-1.24666400	0.78768800	
	O	2.06790400	-0.55863000	-0.42498900	
	H	1.34085200	-0.97491900	0.11167800	
	O	2.06855900	0.70874000	-0.13725700	
s = -1.80298	O	-0.40373600	2.06666100	0.37719200	
s = -1.80298	H	0.42022000	1.55368800	0.42019500	
s = -1.80298	H	-0.18525300	2.87129100	-0.09848400	
s = -1.80298	O	-0.86031800	-1.76890800	-0.10213900	-25, 57, 68, 95, 134, 174, 177, 243, 362, 299, 334, 373, 383,
s = -1.80298	H	-1.54701000	-1.03227500	-0.28356900	469, 612, 660, 881, 963, 1308, 1325, 1533, 1625,
s = -1.80298	O	-2.24564700	0.31797000	-0.50697600	1641, 1673, 2781, 3247, 3359, 3694, 3926, 3928
s = -1.80298	H	-3.07512200	0.46102800	-0.04612300	
s = -1.80298	H	-1.62430000	1.01926900	-0.19884500	
s = -1.80298	O	-0.08383800	-1.24081200	0.79917700	
s = -1.80298	O	2.10903100	-0.56233500	-0.42522300	
s = -1.80298	H	1.38257700	-0.99791100	0.09250200	
s = -1.80298	O	2.06311800	0.70303800	-0.12774000	
TS_WD2	O	0.44430100	2.07593800	-0.38338300	
TS_WD2	H	-0.39652700	1.59689000	-0.42279100	
TS_WD2	H	0.25747700	2.88969800	0.09040900	
TS_WD2	O	0.80297100	-1.80990600	0.07637100	-2576, 45, 55, 73, 141, 169,
TS_WD2	H	1.44077000	-1.06000500	0.29986700	188, 215, 246, 269, 316, 344,
TS_WD2	O	2.26209700	0.27886600	0.48761000	351, 455, 563, 651, 858, 949,
TS_WD2	H	3.07199500	0.34103600	-0.02339800	1061, 1242, 1460, 1481,
TS_WD2	H	1.67515100	1.00261900	0.17756500	1621, 1632, 1666, 2963,
TS_WD2	O	-0.06663100	-1.23191400	-0.75695300	3437, 3739, 3924, 3932
TS_WD2	O	-1.99492200	-0.51204300	0.40623500	
TS_WD2	H	-1.06582100	-0.94824800	-0.15384400	
TS_WD2	O	-2.07069500	0.72131000	0.17414500	
s = 0.42951	O	-0.43687700	2.07831900	0.38390400	
s = 0.42951	H	0.39372100	1.59684900	0.42940100	
s = 0.42951	H	-0.24877600	2.89222100	-0.08931500	
s = 0.42951	O	-0.81101700	-1.81058900	-0.08345100	-235, -142, -100, -62, 124,
s = 0.42951	H	-1.43042000	-1.07121900	-0.29902300	163, 234, 236, 254, 275, 292,
s = 0.42951	O	-2.26087900	0.28709400	-0.48754500	324, 339, 442, 499, 590, 786,
s = 0.42951	H	-3.06903700	0.34919600	0.02515900	903, 1192, 1373, 1489, 1607,
s = 0.42951	H	-1.67576100	1.00351800	-0.17604700	1628, 1660, 3015, 3298,
s = 0.42951	O	0.07475500	-1.22665400	0.75939100	3556, 3865, 3931, 3959
s = 0.42951	O	2.00147700	-0.50249700	-0.40993600	
s = 0.42951	H	0.89475600	-1.02390300	0.23594800	
s = 0.42951	O	2.07448100	0.70599400	-0.17812800	
s = 0.94445	O	-0.42334500	2.08549300	0.38424200	
s = 0.94445	H	0.39473700	1.58950700	0.45588300	
s = 0.94445	H	-0.21979200	2.89560900	-0.08824500	
s = 0.94445	O	-0.83489200	-1.81755000	-0.10033600	-374, -232, -121, -107, -73,
s = 0.94445	H	-1.44202600	-1.07196900	-0.30234500	30, 110, 143, 200, 221, 253,
s = 0.94445	O	-2.26160900	0.30866000	-0.49358100	278, 293, 341, 411, 439, 770,
s = 0.94445	H	-3.06719000	0.36888100	0.02328100	856, 1111, 1366, 1595, 1600,
s = 0.94445	H	-1.67242400	1.01450600	-0.17108900	1649, 1727, 3382, 3587,
s = 0.94445	O	0.06072600	-1.21932600	0.78582400	3879, 3932, 3934, 3979
s = 0.94445	O	2.02266600	-0.48926700	-0.41744500	
s = 0.94445	H	0.83521300	-1.15154900	0.24325000	
s = 0.94445	O	2.08289000	0.67636700	-0.17879600	
s = 1.41694	O	-0.41343500	2.09336100	0.38562800	
s = 1.41694	H	0.39138700	1.58090600	0.48884100	
s = 1.41694	H	-0.18055300	2.89496700	-0.08745900	
s = 1.41694	O	-0.85581700	-1.82360100	-0.11257400	-218, -152, -111, -97, -57, 26,
s = 1.41694	H	-1.45367300	-1.07000700	-0.31542800	122, 130, 168, 209, 324, 267,
s = 1.41694	O	-2.26474200	0.33035500	-0.50236000	294, 336, 404, 422, 772, 850,
s = 1.41694	H	-3.06785300	0.38679600	0.01886400	1065, 1370, 1593, 1594,
s = 1.41694	H	-1.66942700	1.02640600	-0.16976500	1645, 1761, 3383, 3590,
s = 1.41694	O	0.03603100	-1.21638300	0.80423400	3874, 3930, 3974, 3976
s = 1.41694	O	2.04788800	-0.49094700	-0.43113000	
s = 1.41694	H	0.84374900	-1.29521400	0.30911200	
s = 1.41694	O	2.09212100	0.66673200	-0.17431900	
s = 1.88947	O	-0.40973000	2.10019100	0.38957900	-146, -105, -93, -56, 56, 94,
s = 1.88947	H	0.37826300	1.56766800	0.52223600	132, 145, 158, 214, 243, 261,
s = 1.88947	H	-0.14197600	2.88952400	-0.08554400	297, 327, 402, 434, 775, 844,
s = 1.88947	O	-0.867776400	-1.82860700	-0.12215800	1051, 1360, 1595, 1597,
s = 1.88947	H	-1.45399400	-1.06836500	-0.33550200	1644, 1762, 3387, 3593,
s = 1.88947	O	-2.26949200	0.34644600	-0.51123500	3865, 3930, 3958, 3967,
s = 1.88947	H	-3.06948800	0.39762600	0.01536500	

	H	-1.67107600	1.03742500	-0.17352900	
	O	0.01337200	-1.21613300	0.81421600	
	O	2.07235200	-0.48923200	-0.44567800	
	H	0.84957800	-1.44144700	0.41273900	
	O	2.09984800	0.66453200	-0.16919500	
$\text{H}_2\text{O}_2^{***}(\text{H}_2\text{O})_2$	O	-1.48944600	0.44378700	-0.45054000	79, 130, 205, 219, 228, 240, 284, 291, 324, 423, 597, 757, 862, 1045, 1372, 1552, 1625, 1639, 3471, 3600, 3721, 3836, 3941, 3943
	H	-0.67247000	0.95441500	-0.26203600	
	O	-1.27194000	-0.73523200	0.31615200	
	H	-1.82151100	-0.58752300	1.09317900	
	O	0.97901100	1.49487500	0.06847300	
	H	1.28372500	1.93147400	0.86557600	
	H	1.41396900	0.62318300	0.03827000	
	O	1.48027900	-1.20120700	-0.05074500	
	H	1.69162700	-1.65164500	-0.87079600	
	H	0.52143500	-1.28768600	0.06909400	
O_2	O	0.00000000	0.00000000	0.59492100	1758
	O	0.00000000	0.00000000	-0.59492100	

**Coordinates and Frequencies of stationary points and the selected points along
the IRC path in the favorable route of $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction with
 $(\text{H}_2\text{O})_2$ occurring through Channel RWD2**

Species	Coordinates			Frequencies
IM_WD3	O	0.94595700	-1.84034300	-0.62329800
	H	1.25144500	-1.12453600	-1.18945600
	H	1.13435700	-2.66027900	-1.08440500
	O	1.55987400	1.27504700	0.27190200
	H	-0.78137900	0.51259500	-0.75398400
	H	1.06959700	0.66820400	0.94769300
	O	0.24431400	-0.39661000	1.62593600
	H	-0.70198800	-0.23803000	1.46347900
	H	0.45866800	-1.17543200	1.08638600
	O	-2.19570000	0.01746700	0.34453300
s = -0.42382	O	-1.75143900	0.31932400	-0.84280200
	O	0.89315600	1.12730000	-0.83498500
	O	-2.28583500	-0.55892600	-0.82682500
	H	-1.59920100	-1.05970700	-0.36333400
	H	-3.12110900	-0.99714500	-0.65291500
	O	0.31431400	-0.17755800	1.46003400
	H	1.12603800	-0.97796200	-0.35587800
	H	-0.19577300	0.60653900	1.04220200
	O	-1.04669700	1.61605500	0.21682700
	H	-0.47646500	2.03950000	-0.43168700
s = -0.98965	H	-1.67082300	1.05037500	-0.27730500
	O	1.87347800	0.70846200	-0.44533200
	O	1.79628900	-0.47705300	0.93693600
	O	0.09061800	-1.19368000	0.66209700
	O	-2.27935600	-0.51094000	-0.88039300
	H	-1.60317300	-1.03331300	-0.42525000
	H	-3.11976600	-0.95032700	-0.73683000
	O	0.27343600	-0.23452500	1.47194600
	H	1.18288600	-0.97823700	-0.42175300
	H	-0.20761400	0.57251700	1.05899300
s = -1.60207	O	-1.03183700	1.60979100	0.25995000
	H	-0.44738100	2.04692300	-0.36661900
	H	-1.65574900	1.06815000	-0.26104300
	O	1.88511800	0.72020400	-0.40522300
	O	1.84153200	-0.44946300	-0.95688600
	O	0.04245600	-1.22578200	0.65466900
	O	-2.27070700	-0.42675900	-0.95172400
	H	-1.61120600	-0.98389100	-0.51333000
	H	-3.11897200	-0.86357200	-0.85373900
	O	0.22225600	-0.34333400	1.48090100
s = -2.21506	H	1.23764400	-0.96113200	-0.49815700
	H	-0.22750500	0.49789000	1.10237000
	O	-1.01274500	1.59358100	0.34882100
	H	-0.40753300	2.05650700	-0.23834200
	H	-1.63597500	1.09782800	-0.21668600
	O	1.89960200	0.74243800	-0.34982100
	O	1.89060800	-0.39292200	-0.97933300
	O	-0.00857000	-1.27845800	0.60339300
	O	-2.26136400	-0.29851100	-1.02615200
	H	-1.62337000	-0.90782200	-0.62713200
TS_WD3	H	-3.11994200	-0.72429900	-0.98709500
	O	0.16711300	-0.50555500	1.46857200
	H	1.27587800	-0.91618400	-0.58500700
	H	-0.25399200	0.37801100	1.16017700
	O	-0.98775900	1.55797500	0.48873400
	H	-0.35022000	2.04771700	-0.03988800
	H	-1.60944600	1.13498700	-0.13434700
	O	1.91325400	0.77400000	-0.27943100
	O	1.93444200	-0.30904900	-0.99858900
	O	-0.05555000	-1.34541100	0.49852700
TS_WD3	O	2.28889400	0.57598300	-0.80247400
	H	1.59815200	1.06483300	-0.33094300
	H	3.12170200	1.01307900	-0.61459400
	O	-0.33559300	0.15517600	1.45813700
	H	-1.04748400	0.984656500	-0.28334600
	H	0.19332200	-0.61045200	1.04916900

	O	1.05229400	-1.61777000	0.20532100	
	H	0.49454000	-2.04053400	-0.45363100	
	H	1.67774800	-1.04317700	-0.27605000	
	O	-1.86844700	-0.69870000	-0.46915500	
	O	-1.77253000	0.47798600	-0.92530600	
	O	-0.11936600	1.18627400	0.64715100	
s = 0.51859	O	-2.28935300	-0.56878600	-0.80253900	
	H	-1.59646900	-1.05888600	-0.32962700	
	H	-3.12169300	-1.00625100	-0.61446400	
	O	0.34311200	-0.15648400	1.45983100	
	H	0.87414100	-1.05525100	-0.12997900	
	H	-0.18512100	0.59005500	1.06751400	
	O	-1.04977300	1.61899600	0.21550200	
	H	-0.49905100	2.04840800	-0.44309800	
	H	-1.67593200	1.04564300	-0.26574200	
	O	1.86904300	0.68993800	-0.47502200	
	O	1.77494000	-0.45866200	-0.93162000	
	O	0.12754600	-1.19546700	0.62327300	
					3944
s = 0.98936	O	-2.28705200	-0.55046900	-0.81833300	
	H	-1.59853700	-1.04312000	-0.34060200	
	H	-3.12085300	-0.98805700	-0.63719700	
	O	0.34588000	-0.17092500	1.46980300	
	H	0.80223500	-1.14650200	-0.06578400	
	H	-0.19046900	0.56538500	1.08931400	
	O	-1.04788800	1.62089600	0.23715100	
	H	-0.50636500	2.06764200	-0.41691000	
	H	-1.67260500	1.05229300	-0.25078500	
	O	1.87338000	0.68007500	-0.46847500	
	O	1.79069600	-0.42137500	-0.93981700	
	O	0.11080800	-1.22165700	0.59741600	
s= 1.60226	O	-2.28160500	-0.50148400	-0.86062600	
	H	-1.60217600	-1.00511400	-0.38130400	
	H	-3.12005400	-0.93798900	-0.69984200	
	O	0.34378900	-0.24035900	1.47683100	
	H	0.81835800	-1.27502100	-0.03505400	
	H	-0.18561500	0.51230200	1.11910700	
	O	-1.04703300	1.62207800	0.29784100	
	H	-0.52285300	2.11352400	-0.33792400	
	H	-1.66804600	1.07079700	-0.21408700	
	O	1.88688100	0.69604400	-0.43016800	
	O	1.82467400	-0.36487400	-0.96814000	
	O	0.05834300	-1.27121700	0.55290000	
s = 2.21528	O	-2.27587300	-0.43433300	-0.90899900	
	H	-1.60233400	-0.96283700	-0.44945700	
	H	-3.11812300	-0.87109300	-0.77075800	
	O	0.33519100	-0.34701700	1.47147500	
	H	0.82218000	-1.40891700	-0.01193000	
	H	-0.16076900	0.44120300	1.14569000	
	O	-1.04620900	1.61681800	0.38364800	
	H	-0.54303400	2.16619400	-0.22093000	
	H	-1.66268600	1.09250000	-0.16082500	
	O	1.90342500	0.72129100	-0.37986000	
	O	1.85942500	-0.29512100	-0.99799100	
	O	0.00713700	-1.31876900	0.49025300	
$\text{H}_2\text{O}_2^{\bullet\bullet}(\text{H}_2\text{O})_2$	O	-1.48944600	0.44378700	-0.45054000	
	H	-0.67247000	0.95441500	-0.26203600	
	O	-1.27194000	-0.73523200	0.31615200	
	H	-1.82151100	-0.58752300	1.09317900	
	O	0.97901100	1.49487500	0.06847300	
	H	1.28372500	1.93147400	0.86557600	
	H	1.41396900	0.62318300	0.03827000	
	O	1.48027900	-1.20120700	-0.05074500	
	H	1.69162700	-1.65164500	-0.87079600	
	H	0.52143500	-1.28768600	0.06909400	
O_2	O	0.00000000	0.00000000	0.59492100	
	O	0.00000000	0.00000000	-0.59492100	1758

Coordinate and Frequencies of stationary points and the selected points along the IRC path in the favorable route of $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction with $(\text{H}_2\text{O})_3$ occurring through Channel RWT1

Species	Coordinates			Frequencies
IM_WT1	O	0.17941400	-0.88208400	-0.40085300
	H	-0.37207700	-0.79681700	-1.18797000
	H	-0.43483500	-1.24037900	0.27368300
	O	-2.38186400	0.05665800	-1.12473300
	H	-3.04351500	0.45052000	-1.69690200
	H	-1.89043400	0.78839600	-0.70838200
	O	-1.98413000	-1.61527300	1.06672200
	H	-2.49830400	-1.09745500	0.42796100
	H	-2.24333700	-1.31733900	1.94100600
	O	0.41535100	1.75188800	0.54435900
	H	0.65994300	0.85459100	0.20369600
	O	-0.84033900	1.93850600	0.26866900
	O	2.81148800	-1.01975000	-0.30922100
	H	1.85383400	-1.23850800	-0.43231100
	O	2.79617200	0.21967900	0.10245900
TS_WT1	O	0.07604100	-0.98225700	-0.53250400
	H	-0.42834900	-0.81768900	-1.33790100
	H	-0.57683100	-1.32808000	0.10791600
	O	-2.45438000	0.35181100	-0.91731600
	H	-3.09085400	0.95965300	-1.31009900
	H	-1.73148300	0.90247200	-0.53963400
	O	-2.11405300	-1.63174300	0.94319800
	H	-2.59223000	-0.95568200	0.42817500
	H	-2.31232300	-1.47123000	1.86971200
	O	0.69821900	1.70026100	0.56040100
	H	0.90267600	0.80168200	0.21134500
	O	-0.52184900	2.00105700	0.23125700
	O	2.67587600	-1.14471500	-0.26713500
	H	1.71745500	-1.35019700	-0.46105200
	O	2.65413900	0.11296900	0.11104100
IM_WT2	O	2.58281700	-1.02775200	0.45279100
	H	3.19220900	-1.59728400	-0.02048400
	H	2.58036300	-0.14105500	0.00388300
	O	-0.14813600	1.82332000	0.55855600
	H	-0.38471300	2.54949800	1.13804000
	H	-0.96528800	1.32132800	0.39756600
	O	2.24558900	1.34792900	-0.63271400
	H	1.38564700	1.58133700	-0.22468300
	H	2.09525300	1.37506500	-1.58004900
	O	-2.80202300	-0.61152900	-0.35157500
	H	-1.86394000	-0.89557000	-0.55547200
	O	-2.67639500	0.57008800	0.18137100
	O	0.11286700	-1.50064000	0.48251600
	H	1.14081000	-1.40356600	0.52336700
	O	-0.21226200	-0.95013500	-0.65121600
$s = -0.36467$	O	1.84731400	-1.05427800	1.06169900
	H	2.63883400	-1.44407100	1.43687400
	H	2.10123100	-0.19880400	0.62954600
	O	-0.15435100	2.38375800	-0.22501000
	H	-0.35343700	3.18659600	0.26095200
	H	-0.88562600	1.77084900	-0.04084200
	O	2.31519400	1.22301800	-0.21951800
	H	1.44618700	1.67782100	-0.21721400
	H	2.54647200	1.11130600	-1.14406600
	O	-2.33373400	-0.60634000	0.32863200
	H	-1.52862300	-0.79790700	-0.25301500
	O	-2.38626200	0.65887000	0.51097100
	O	0.20897000	-2.08982700	-0.60467700
	H	0.91186000	-1.80749900	0.08601200
	O	-0.35674500	-0.95248700	-0.94687700
$s = -0.79381$	O	1.84680600	-1.04520300	1.06521800
	H	2.63781200	-1.43007700	1.44658800
	H	2.09722400	-0.18503200	0.63930500
	O	-0.16538700	2.38034500	-0.22762800
	H	-0.37006500	3.18398300	0.25454700
	H	-0.89536000	1.76466800	-0.04794200

	O	2.30898300	1.23316700	-0.21081400	3040, 3241, 3467, 3677, 3925, 3937, 3939
	H	1.43805600	1.68454900	-0.21150900	
	H	2.54648800	1.12771300	-1.13446400	
	O	-2.36018800	-0.62355600	0.33674800	
	H	-1.60379000	-0.81443200	-0.28854300	
	O	-2.38772600	0.66072900	0.50230300	
	O	0.22462100	-2.08609800	-0.59647800	
	H	0.94963100	-1.80072200	0.07176400	
	O	-0.31710700	-0.96071600	-0.96056700	
s = -1.39468	O	1.85141100	-1.03078200	1.06422500	
	H	2.64324700	-1.40092700	1.45809300	
	H	2.09214100	-0.16474900	0.64312500	
	O	-0.18391800	2.37388100	-0.22960100	
	H	-0.40705000	3.17257500	0.25248300	
	H	-0.90723000	1.74689900	-0.06571900	
	O	2.29738800	1.25188900	-0.19606600	
	H	1.42131300	1.69320600	-0.20199500	
	H	2.54169200	1.15038300	-1.11838100	
	O	-2.40437100	-0.64079200	0.34413700	
	H	-1.69337500	-0.85344000	-0.31693100	
	O	-2.38833300	0.65007300	0.49058400	
	O	0.25262600	-2.08761500	-0.58201000	
	H	0.99286900	-1.79762900	0.06689700	
	O	-0.26025400	-0.95994400	-0.98096500	
s = -1.99555	O	1.86785800	-1.01783300	1.05671200	
	H	2.66440700	-1.36788600	1.45896200	
	H	2.09117500	-0.14620600	0.63529200	
	O	-0.20074500	2.36357500	-0.23348800	
	H	-0.44835300	3.14908000	0.25833800	
	H	-0.90864100	1.71647800	-0.08323000	
	O	2.28569200	1.27091800	-0.18272400	
	H	1.40569800	1.70477500	-0.19067300	
	H	2.52923600	1.16682800	-1.10503800	
	O	-2.45582900	-0.65193100	0.33965700	
	H	-1.74519700	-0.88784000	-0.30749800	
	O	-2.38837500	0.63852500	0.48638700	
	O	0.27398800	-2.08875300	-0.56669700	
	H	1.01733400	-1.80123200	0.07919500	
	O	-0.20829700	-0.95625000	-0.99301600	
TS_WT2	O	1.84890700	-1.05284100	1.06105900	
	H	2.64159300	-1.44173500	1.43394600	
	H	2.10251200	-0.20081200	0.62720700	
	O	-0.15672700	2.38479200	-0.22340700	
	H	-0.35577900	3.18704500	0.26369700	
	H	-0.88318600	1.77149800	-0.04056000	
	O	2.31369300	1.22508100	-0.22133900	
	H	1.44520200	1.67687300	-0.21891900	
	H	2.54276800	1.11093900	-1.14615100	
	O	-2.33184700	-0.59605100	0.33191000	
	H	-1.39360000	-0.83202200	-0.32074300	
	O	-2.38793200	0.64643000	0.51358000	
	O	0.21105200	-2.09642900	-0.60386200	
	H	0.89720400	-1.81350900	0.08360200	
	O	-0.37173700	-0.94326700	-0.94320000	
s = 0.32189	O	1.84996500	-1.04961800	1.06220000	
	H	2.64335300	-1.43704600	1.43401900	
	H	2.10224000	-0.20097100	0.62751000	
	O	-0.16097000	2.38521200	-0.22279400	
	H	-0.36063700	3.18752500	0.26437700	
	H	-0.88047700	1.77239000	-0.04254300	
	O	2.31122900	1.22873800	-0.22120600	
	H	1.44390200	1.67650100	-0.21969800	
	H	2.53930700	1.11273700	-1.14603600	
	O	-2.33628700	-0.59009500	0.33697900	
	H	-1.26386900	-0.86779600	-0.39814800	
	O	-2.38999500	0.63610700	0.51395000	
	O	0.21488100	-2.10081700	-0.60148900	
	H	0.88793600	-1.81836200	0.07544900	
	O	-0.37779200	-0.93764800	-0.94200700	
s = 0.87969	O	1.85424600	-1.03906000	1.07092600	
	H	2.65115000	-1.42153300	1.43990300	
	H	2.10478900	-0.19681500	0.62821100	
	O	-0.17043900	2.38831500	-0.222301100	
	H	-0.37797200	3.18699500	0.26654000	
	H	-0.87724600	1.76400100	-0.05121900	

	O	2.30736900	1.24097700	-0.21686900	3413, 3596, 3885, 3918, 3925, 3948, 3985
	H	1.43586700	1.67635400	-0.22060200	
	H	2.53266400	1.11419900	-1.14106000	
	O	-2.35797200	-0.57464800	0.35115500	
	H	-1.17978500	-0.96914100	-0.47553400	
	O	-2.39652300	0.60740700	0.50915600	
	O	0.23124500	-2.12135000	-0.59736000	
	H	0.89277100	-1.82548200	0.06908800	
	O	-0.36570600	-0.91771400	-0.95841300	
s = 1.52347	O	1.86158100	-1.02277400	1.09122600	
	H	2.66433500	-1.39658000	1.45683100	
	H	2.10659900	-0.18504500	0.63738900	
	O	-0.17907200	2.39410700	-0.23071800	
	H	-0.40874500	3.18041900	0.26876700	
	H	-0.86674100	1.74597700	-0.06724000	
	O	2.30567400	1.25603900	-0.21254000	
	H	1.42857000	1.68016400	-0.22260900	
	H	2.52579200	1.10599000	-1.13468700	
	O	-2.39672200	-0.57981600	0.37361500	
	H	-1.20865700	-1.05352600	-0.64115800	
	O	-2.40773700	0.60013400	0.50424200	
	O	0.25343600	-2.14396100	-0.59448000	
	H	0.90428600	-1.83760700	0.07866300	
	O	-0.33034000	-0.90870300	-0.97834000	
s = 1.95267	O	1.86477300	-1.01623500	1.10509700	
	H	2.67084900	-1.38491700	1.46873200	
	H	2.10574600	-0.17968800	0.64739900	
	O	-0.17907200	2.39853300	-0.23742100	
	H	-0.42424900	3.17308300	0.27294000	
	H	-0.84959500	1.73132700	-0.07596600	
	O	2.30780800	1.26017400	-0.21179200	
	H	1.43184400	1.68671700	-0.22419100	
	H	2.52241200	1.09410800	-1.13257600	
	O	-2.42056700	-0.57970300	0.38905400	
	H	-1.22663500	-1.09769600	-0.79156800	
	O	-2.41404700	0.60224800	0.50274300	
	O	0.26082600	-2.15326200	-0.59298600	
	H	0.89927700	-1.84513000	0.09132700	
	O	-0.31092700	-0.90898100	-0.98670700	
O ₂	O	0.00000000	0.00000000	0.59492100	1758
H ₂ O ₂ •••(H ₂ O) ₃	O	0.00000000	0.00000000	-0.59492100	
	O	-0.60802400	1.85546600	0.49296600	
	H	-1.31529100	1.21985300	0.25510500	
	O	-2.20863700	-0.21970400	-0.21896300	
	H	-1.53484700	-0.92085100	-0.10653700	
	O	-0.18273700	-2.03677800	0.15092600	
	H	-0.18276500	-2.49615700	0.99308400	
	O	1.36488000	0.57180000	-0.78523800	
	H	0.72657500	1.15851000	-0.31625700	
	H	-0.96260600	2.73786700	0.37625100	
	H	-2.52021100	-0.29980600	-1.12233800	
	H	0.64148100	-1.52570500	0.13174600	
	O	1.92106800	-0.16251200	0.30393700	
	H	2.85526900	0.06011700	0.23992600	

**Coordinates and Frequencies of stationary points and the selected points along
the IRC path in the favorable route of $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + {}^3\text{O}_2$ reaction with
 $(\text{H}_2\text{O})_3$ occurring through Channel RWT2**

Species	Coordinates				Frequencies
IM_MT3	O	1.05361700	-1.46482200	-0.97101700	
	H	1.48684200	-0.57619900	-0.92282100	
	O	2.24365400	0.88556800	-0.46283400	
	H	1.93175800	0.78423000	0.45249200	35 , 45, 61, 81, 117, 140,
	O	1.04508800	-0.18966600	1.78522700	151, 171, 213, 222, 235,
	H	0.92481500	-0.01202300	2.72009500	244, 258, 309, 334, 397,
	O	-1.43312500	-1.37173200	-0.57883600	426, 450, 458, 568, 641,
	H	-0.42056100	-1.43034100	-0.79412000	662, 914, 1069, 1284, 1332,
	H	1.51713200	-2.00664600	-0.32619500	1514 ,1613, 1638, 1656,
	H	1.76189400	1.64073900	-0.81267400	1696, 2554, 3297, 3502,
	H	0.17962400	-0.46600000	1.44101300	3656, 3690, 3896, 3900,
	O	-1.49389700	-0.93162200	0.64370500	3941
	O	-1.55730700	1.74818000	0.04568700	
	H	-1.91636000	0.87594400	0.32183200	
	O	-0.54117300	1.47288200	-0.72188500	
s = -0.26738	O	0.92097600	-0.90974700	-1.51042800	
	H	1.27623700	-0.03271400	-1.23338700	
	O	1.91794100	1.30145500	-0.30719200	
	H	1.85410400	0.81634900	0.53022400	-54, 17, 68, 74, 102, 136,
	O	1.47206100	-0.85718200	1.41560900	150, 199, 211, 230, 252,
	H	1.65472900	-1.16895700	2.30432200	293, 324, 335, 358, 376,
	O	-1.47180300	-1.07175200	-0.67823400	407, 451, 525, 606, 633,
	H	-0.52155400	-1.01805300	-1.08501800	731, 874, 1107, 1181, 1340,
	H	1.49709900	-1.55106000	-1.08287600	1595, 1608, 1631, 1642,
	H	1.29604100	2.03229000	-0.24552000	1689, 2342, 2560, 3380,
	H	0.54380400	-1.06833600	1.22881900	3693, 3731, 3884, 3909,
	O	-1.28438600	-1.06997100	0.62382600	3934
	O	-1.26223000	1.32191700	0.77353500	
	H	-1.37348400	0.30550400	0.90443400	
	O	-1.07093100	1.49590300	-0.48224200	
s = -1.0262	O	0.91112400	-0.93383300	-1.49102900	
	H	1.27003400	-0.05411800	-1.22354700	
	O	1.91835800	1.28934200	-0.33057600	
	H	1.85829200	0.82315000	0.51779800	23, 34, 70, 79, 124, 143,
	O	1.47078400	-0.83920400	1.42895600	199, 209, 228, 250, 263,
	H	1.64676900	-1.13261500	2.32523600	293, 304, 354, 383, 407,
	O	-1.47084200	-1.10610200	-0.66331100	451, 528, 535, 632, 670,
	H	-0.51956500	-1.04247900	-1.07485500	876, 1100, 1273, 1321,
	H	1.48235800	-1.57144700	-1.05122200	1554, 1610, 1632, 1642,
	H	1.27895500	2.00694800	-0.29077300	1692, 2526, 3022, 3357,
	H	0.53968300	-1.04147300	1.24417500	3686, 3732, 3881, 3900,
	O	-1.28253000	-1.11451800	0.62743800	3932
	O	-1.26111400	1.39861400	0.76583300	
	H	-1.43466000	0.42781600	0.93127600	
	O	-1.05110300	1.50372900	-0.50957300	
s = -1.56109	O	0.90078000	-0.95478200	-1.47632800	
	H	1.26605500	-0.07536200	-1.21525800	
	O	1.92432500	1.26973500	-0.34518800	
	H	1.86395300	0.81592300	0.50989200	18, 38, 66, 74, 125, 142,
	O	1.46205100	-0.83415000	1.43941100	174, 199, 203, 221, 228,
	H	1.62733600	-1.11747800	2.34091900	263, 270, 301, 350, 381,
	O	-1.47957000	-1.13265800	-0.65586100	409, 445, 482, 529, 631,
	H	-0.52974600	-1.06282200	-1.06916900	668, 877, 1095, 1280, 1324,
	H	1.46650600	-1.59322700	-1.03066900	1536, 1610, 1632, 1641,
	H	1.28401300	1.98721300	-0.31666800	1692, 2536, 3226, 3348,
	H	0.53105800	-1.03289300	1.24821300	3682, 3731, 3881, 3895,
	O	-1.28705300	-1.13286100	0.63239400	3931
	O	-1.25525800	1.45681300	0.75380700	
	H	-1.46698100	0.50522700	0.93533400	
	O	-1.02054900	1.52458100	-0.52356000	
s = -2.09678	O	0.88399200	-0.98336600	-1.46139100	21, 41, 59, 72, 131, 144,
	H	1.25965700	-0.10631300	-1.20635300	168, 185, 199, 215, 231,
	O	1.94120100	1.23354400	-0.35576600	265, 273, 300, 341, 383,
	H	1.87414800	0.79214900	0.50533200	412, 439, 475, 531, 631,
	O	1.44129300	-0.84078900	1.45191800	666, 878, 1084, 1279, 1328,
	H	1.59100200	-1.11623900	2.35855200	1527, 1608, 1631, 1640,

	O -1.49854700 -1.15106800 -0.65041200 H -0.54915100 -1.08356300 -1.06387000 H 1.44214000 -1.62532800 -1.01129100 H 1.31201700 1.96119400 -0.33712800 H 0.50959000 -1.02799800 1.25142400 O -1.30384700 -1.13423900 0.63666200 O -1.23909000 1.52003500 0.73732900 H -1.49390100 0.58486200 0.92528800 O -0.96818900 1.55853700 -0.53608400	1692, 2544, 3342, 3381, 3677, 3731, 3881, 3893, 3932
TS_MT3	O -0.91988300 -0.90507400 1.51512100 H -1.27807300 -0.03154800 1.23649400 O -1.92004400 1.30027400 0.30318400 H -1.85580200 0.80965000 -0.53126400 O -1.47110500 -0.86404600 -1.41145000 H -1.65401100 -1.18080500 -2.29833600 O 1.47592100 -1.06282800 0.68697600 H 0.53183300 -1.01535900 1.08671900 H -1.49415600 -1.54972200 1.09054500 H -1.30551600 2.03605500 0.23554800 H -0.54317700 -1.07739700 -1.22269600 O 1.28562800 -1.05564200 -0.63020900 O 1.25850300 1.31325700 -0.76980800 H 1.35472500 0.21341400 -0.89016800 O 1.07150300 1.49852200 0.46783100	-1623, 40, 63, 79, 97, 132, 147, 189, 198, 222, 235, 263, 295, 352, 376, 393, 399, 457, 522, 619, 643, 712, 865, 973, 1119, 1289, 1454, 1606, 1625, 1639, 1686, 1704, 2677, 3408, 3683, 3726, 3887, 3917, 3935
	O 0.91495400 -0.90063100 -1.52090000 H 1.27954900 -0.03546500 -1.24044800 O 1.92689500 1.29345800 -0.29853700 H 1.86137200 0.79565400 0.53279000 O 1.46770600 -0.87665400 1.40584300 H 1.64969400 -1.19983400 2.29049300 O -1.48373500 -1.04842500 -0.69938500 H -0.55879600 -1.01190300 -1.08506100 H 1.48418500 -1.55117600 -1.09962300 H 1.32274300 2.03530000 -0.22488600 H 0.53685200 -1.08851600 1.21443100 O -1.28940300 -1.04070000 0.63789700 O -1.24821900 1.32520800 0.76514000 H 1.35330800 -0.01787500 0.87814500 O -1.06598300 1.50697000 -0.44828800	-127, -62, 41, 77, 107, 115, 161, 198, 239, 253, 272, 277, 376, 253, 272, 277, 324, 352, 366, 376, 440, 484, 497, 602, 681, 833, 887, 1065, 1150, 1374, 1609, 1629, 1639, 1664, 1688, 2136, 3070, 3492, 3631, 3703, 3895, 3934, 3934
	O 0.91680400 -0.90272700 -1.52377400 H 1.29092800 -0.04302400 -1.24598500 O 1.93357400 1.28686800 -0.29625900 H 1.86437800 0.78141900 0.53049900 O 1.46261500 -0.88224400 1.40540400 H 1.64315100 -1.21069600 2.28832900 O -1.49702700 -1.03974800 -0.71915100 H -0.57403800 -1.02047900 -1.08522700 H 1.47819000 -1.55906900 -1.10157500 H 1.35005700 2.04327000 -0.21373500 H 0.53461200 -1.10228500 1.20640300 O -1.28676300 -1.05281200 0.65610700 O -1.23797900 1.35777200 0.74507100 H -1.42055400 -0.13921400 0.92397900 O -1.06206500 1.51415100 -0.43023300	-167, -86, -54, 56, 90, 102, ,135, 165, 185, 194, 230, 248, 253, 265, 329, 355, 375, 448, 477, 481, 585, 726, 817, 1008, 1114, 1432, 1596, 1614, 1640, 1679, 1683, 3210, 3524, 3622, 3667, 3696, 3899, 3934, 3939
	O 0.92450300 -0.90627600 -1.52746400 H 1.30560200 -0.05017200 -1.24942000 O 1.94518800 1.27640800 -0.28609100 H 1.86391900 0.76176200 0.53408400 O 1.45193500 -0.89294900 1.40716100 H 1.62671200 -1.23130700 2.28733200 O -1.51435500 -1.02843800 -0.73294000 H -0.58866300 -1.01188600 -1.09205300 H 1.47600900 -1.56905400 -1.10256800 H 1.39327100 2.05405400 -0.18711900 H 0.52597400 -1.11091200 1.19714500 O -1.28488700 -1.08249300 0.66067000 O -1.22819600 1.39994500 0.74070700 H -1.55306900 -0.21185000 0.96405100 O -1.05040700 1.52997200 -0.43097400	-97, -62, 18, 71, 115, 122, 141, 178, 193, 199, 220, 245, 255, 267, 320, 351, 365, 434, 467, 482, 583, 720, 814, 989, 1061, 1395, 1591, 1612, 1639, 1680, 1726, 3218, 3532, 3628, 3690, 3808, 3901, 3936, 3937
	O 0.92812500 -0.91714800 -1.53123800 H 1.31700700 -0.06489200 -1.25391600 O 1.96471900 1.25530800 -0.27560200 H 1.86827800 0.73464300 0.53918800 O 1.43629700 -0.90919000 1.40959000 H 1.60067400 -1.25835100 2.28743600	-75, -53, 22, 68, 116, 121, 129, 183, 191, 194, 218, 228, 246, 250, 315, 337, 347, 402, 439, 476, 572, 700, 804, 961, 1048, 1382, 1594, 1613, 1636, 1679,

	O	-1.53746800	-1.01452700	-0.73772300	1735, 3230, 3543, 3630,
	H	-0.61289000	-0.99287800	-1.09797200	3684, 3843, 3901, 3935,
	H	1.46671200	-1.58523800	-1.09829600	3943
	H	1.45260600	2.05743100	-0.16007000	
	H	0.50691500	-1.10477100	1.19427000	
	O	-1.29079300	-1.10383600	0.65855000	
	O	-1.21074800	1.44886100	0.73692400	
	H	-1.68553100	-0.29337100	0.99234900	
	O	-1.02935400	1.55396200	-0.43587500	
O ₂	O	0.00000000	0.00000000	0.59492100	1758
O	O	0.00000000	0.00000000	-0.59492100	
H ₂ O ₂ •••(H ₂ O) ₃	O	-0.60802400	1.85546600	0.49296600	
H	H	-1.31529100	1.21985300	0.25510500	
O	O	-2.20863700	-0.21970400	-0.21896300	
H	H	-1.53484700	-0.92085100	-0.10653700	
O	O	-0.18273700	-2.03677800	0.15092600	41, 55, 83, 120, 181, 188,
H	H	-0.18276500	-2.49615700	0.99308400	223, 236, 240, 249, 276,
O	O	1.36488000	0.57180000	-0.78523800	295, 331, 508, 592, 715,
H	H	0.72657500	1.15851000	-0.31625700	807, 911, 1043, 1352, 1561,
H	H	-0.96260600	2.73786700	0.37625100	1632, 1642, 1662
H	H	-2.52021100	-0.29980600	-1.12233800	
H	H	0.64148100	-1.52570500	0.13174600	
O	O	1.92106800	-0.16251200	0.30393700	
H	H	2.85526900	0.06011700	0.23992600	