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Effect of NH_3 and HCOOH on $H_2O_2 + HO \rightarrow HO_2 + H_2O$ reaction in the troposphere: competition between one-step and stepwise mechanism

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Table S1 Energy barriers (Δ*E*) for the H_2O_2 + HO → HO_2 + H_2O reaction at different theoretical methods with zero-point correction involved and unsigned error (UE) (in kcal·mol^{-1})

Methods	ΔE^a	ΔE^b	ΔE^c	UE
W3X-l//M06-2X/aug-cc-pVTZ	-13.4	2.7	-35.1	0.00
W2X//M06-2X/aug-cc-pVTZ	-13.2	3.2	-35.0	0.26
CCSD(T)-F12a/pVDZ-F12//M06-2X/aug-cc-pVTZ	-13.7	2.6	-35.4	0.23

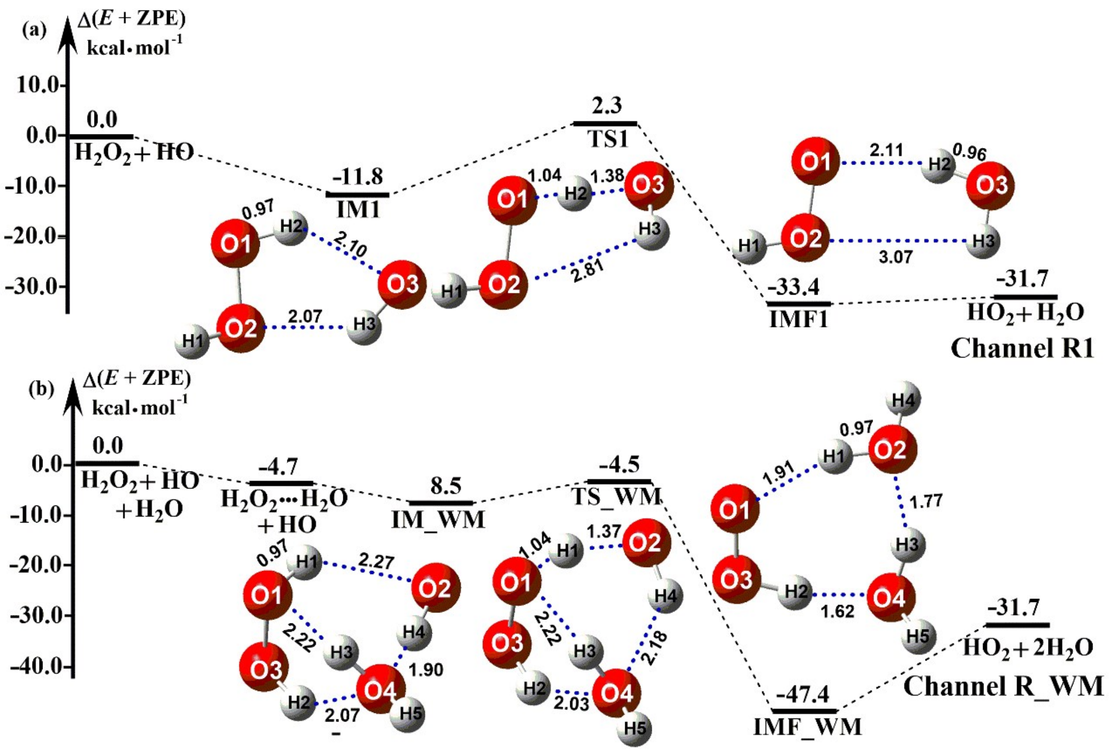

Fig. S1 Schematic potential energy diagrams for the H_2O_2 + HO → HO_2 + H_2O reaction without and with H_2O at the CCSD(T)-F12a/cc-pVDZ-F12//M06-2X/aug-cc-pVTZ level

The H_2O_2 + HO → HO_2 + H_2O reaction were investigated theoretically in the previous reports.[1-6] In this study, we have reinvestigated this reaction at the CCSD(T)-F12a/cc-pVDZ -F12//M06-2X/aug-cc-pVTZ level in order to confirm the catalytic effect of catalyst *X* (*X* = NH_3 and HCOOH). As seen, beginning with H_2O_2 + HO reactants, five-membered ring (O2···H3-O3···H2-O1) complex IM1 has been formed with two weak hydrogen bonds involved. The stabilization energy of IM1 is 11.8 kcal·mol^{-1}. After complex IM1, the reaction proceeded via H-abstraction transition state TS1 to form the post-reactive complex IMF1. From an energetic standpoint, transition state TS1 was predicted to be 2.3 kcal·mol^{-1} above the reactants, which was slightly different from the corresponding value (1.5 kcal·mol^{-1}) obtained by our previous result. The complex IMF1 then dissociates to produce the final products H_2O + HO_2, which lies 31.7 kcal·mol^{-1} below the energy of H_2O_2 + HO reactants.

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[5] R. J. Buszek, M. Torrent-Sucarrat, J. M. Anglada and J. S. Francisco, *J. Phys. Chem. A*, 2012, **116**, 5821.
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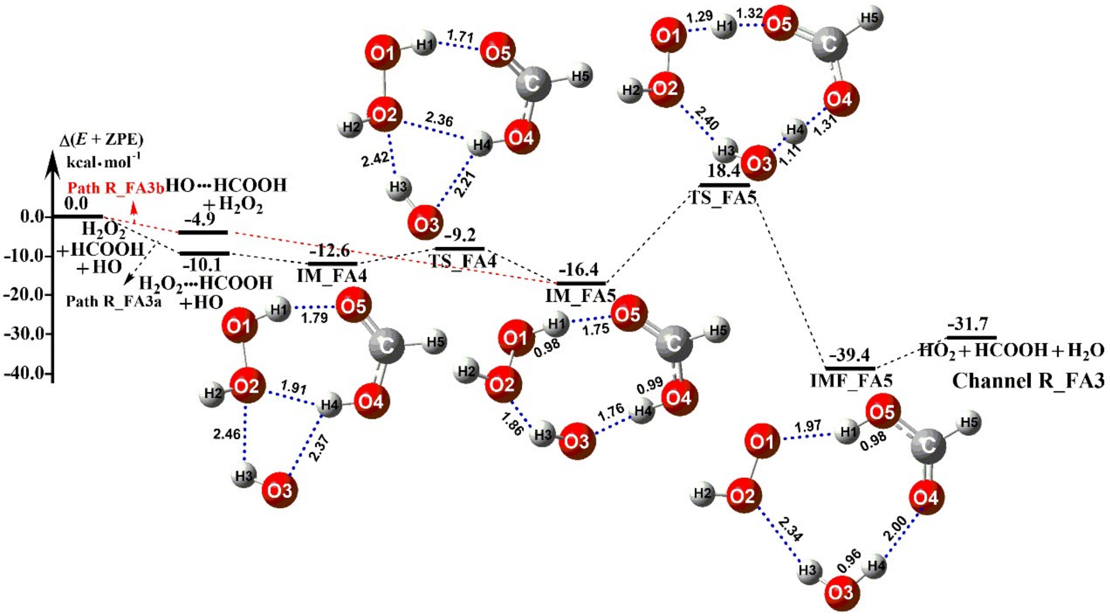
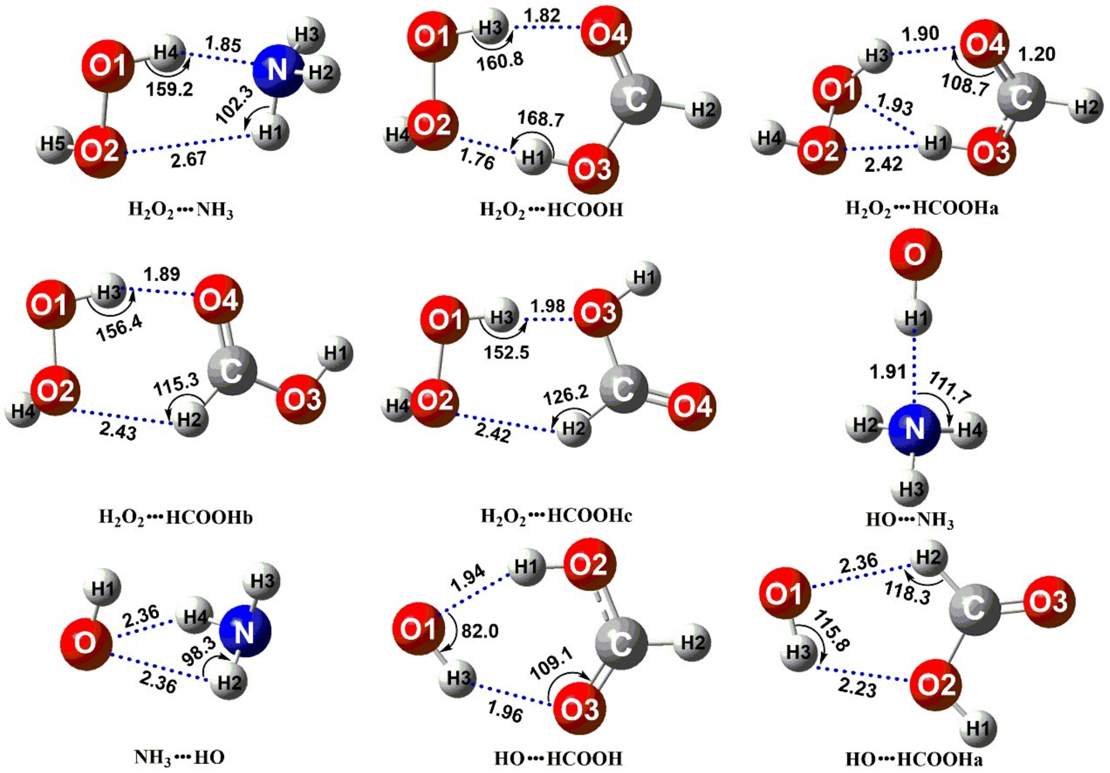


Fig. S2 Schematic potential energy diagrams for less favorable channels involved in HCOOH catalyzed H_2O_2 + HO → HO_2 + H_2O reaction at the CCSD(T)-F12a/cc-pVDZ-F12//M06-2X /aug-cc-pVTZ level



H_2O_2···NH_3 H_2O_2···HCOOH H_2O_2···HCOOHa

H_2O_2···HCOOHb H_2O_2···HCOOHc HO···NH_3

NH_3···HO HO···HCOOH HO···HCOOHa

Fig. S3 Optimized geometries of all complexes for the H_2O_2 + HO → HO_2 + H_2O reaction with acidic (HCOOH) and basic (NH_3) catalysts at the M06-2X/aug-cc-pVTZ level

Table S2 Relative energies ((ΔE), (ΔE + ZPE)), enthalpies (ΔH) and free energies (ΔG) for the possible stable complexes between H_2O_2 (or HO) and the catalyst X (X = NH_3 and HCOOH) at the CCSD(T)-F12a/cc-pVDZ-F12//M06-2X/aug-cc-pVTZ level

Species	ΔE(298 K) (kcal·mol^{-1})	ΔH(298 K) (kcal·mol^{-1})	ΔG(298 K) (kcal·mol^{-1})	Δ(E + ZPE) (298 K) (kcal·mol^{-1})
$H_2O_2 + NH_3$	0.0	0.0	0.0	0.0
$H_2O_2\cdots NH_3$	-8.6	-6.9	0.8	-6.6
$HO + NH_3$	0.0	0.0	0.0	0.0
$HO\cdots NH_3$	-7.8	-6.3	1.1	-5.5
$NH_3\cdots HO$	-1.6	-0.4	6.2	0.0
H_2O_2 + HCOOH	0.0	0.0	0.0	0.0
$H_2O_2\cdots$HCOOH	-12.1	-10.5	-0.5	-10.1
$H_2O_2\cdots$HCOOHa	-9.6	-8.0	1.5	-7.8
$H_2O_2\cdots$HCOOHb	-7.2	-5.6	2.9	-5.7
$H_2O_2\cdots$HCOOHc	-4.8	-3.3	4.7	-3.5
HO + HCOOH	0.0	0.0	0.0	0.0
HO···HCOOH	-5.5	-4.1	4.4	-4.9
HO···HCOOHa	-3.2	-2.1	4.6	-2.0

Table S3 Equilibrium constants ($cm^3\cdot molecule^{-1}$) for the formation of two-body complexes between H_2O_2 (or HO) and the catalyst *X* (*X* = NH_3 and HCOOH) within the temperature range of 213-320 K

T/K	$K_{eq}(H_2O_2\cdots H_2O)$	$K_{eq}(H_2O_2\cdots NH_3)$	$K_{eq}(HO\cdots NH_3)$	$K_{eq}(NH_3\cdots HO)$	$K_{eq}(H_2O_2\cdots HCOOH)$
213	5.05×10^{-23}	2.01×10^{-20}	6.20×10^{-21}	1.22×10^{-25}	2.13×10^{-18}
230	3.20×10^{-23}	8.90×10^{-21}	3.36×10^{-21}	1.60×10^{-25}	5.05×10^{-19}
259	1.71×10^{-23}	2.88×10^{-21}	1.43×10^{-21}	2.37×10^{-25}	6.80×10^{-20}
280	1.20×10^{-23}	1.49×10^{-21}	8.65×10^{-22}	3.04×10^{-25}	2.10×10^{-20}
290	1.03×10^{-23}	1.13×10^{-21}	7.00×10^{-22}	3.39×10^{-25}	1.28×10^{-20}
298	9.20×10^{-24}	9.20×10^{-22}	5.95×10^{-22}	3.69×10^{-25}	8.75×10^{-21}
Con.	7.05×10^{3} (100% RH)	65.50 (2900 ppbv) 0.23 (10 ppbv)	0.42 (2900 ppbv) 1.49×10^{-3} (10 ppbv) (1.35×10^{-3})[a]	2.62×10^{-4} (2900 ppbv) 9.2×10^{-7} (10 ppbv)	2.10 (High) 0.17 (Average)
300	8.95×10^{-24}	8.75×10^{-22}	5.75×10^{-22}	3.76×10^{-25}	8.00×10^{-21}
310	7.85×10^{-24}	6.90×10^{-22}	4.79×10^{-22}	4.15×10^{-25}	5.20×10^{-21}
320	7.00×10^{-24}	5.55×10^{-22}	4.04×10^{-22}	4.57×10^{-25}	3.49×10^{-21}

T/K	$K_{eq}(H_2O_2\cdots HCOOHa)$	$K_{eq}(H_2O_2\cdots HCOOHb)$	$K_{eq}(H_2O_2\cdots HCOOHc)$	$K_{eq}(HO\cdots HCOOH)$	$K_{eq}(HO\cdots HCOOHa)$
213	2.11×10^{-20}	7.10×10^{-22}	1.59×10^{-23}	5.05×10^{-23}	1.72×10^{-23}
230	7.50×10^{-21}	3.67×10^{-22}	1.14×10^{-23}	3.80×10^{-23}	1.55×10^{-23}
259	1.80×10^{-21}	1.49×10^{-22}	7.35×10^{-24}	2.57×10^{-23}	1.36×10^{-23}
280	7.80×10^{-22}	8.80×10^{-23}	5.80×10^{-24}	2.05×10^{-23}	1.28×10^{-23}
290	5.50×10^{-22}	7.05×10^{-23}	5.25×10^{-24}	1.86×10^{-23}	1.25×10^{-23}
298	4.22×10^{-22}	6.00×10^{-23}	4.88×10^{-24}	1.74×10^{-23}	1.23×10^{-23}
Con.	0.10 (High) 8.00×10^{-3} (Average)	0.01 (High) 1.14×10^{-3} (Average)	1.17×10^{-3} (High) 9.25×10^{-5} (Average)	4.17×10^{-5} (High) 3.30×10^{-6} (Average) (4.90×10^{-5})[a]	2.95×10^{-5} (High) 2.34×10^{-6} (Average)
300	3.96×10^{-22}	5.80×10^{-23}	4.80×10^{-24}	1.71×10^{-23}	1.23×10^{-23}
310	2.93×10^{-22}	4.81×10^{-23}	4.43×10^{-24}	1.58×10^{-23}	1.21×10^{-23}
320	2.21×10^{-22}	4.05×10^{-23}	4.13×10^{-24}	1.47×10^{-23}	1.20×10^{-23}

[a] The Value was from Ref (S. Mallick, S. Sarkar, P. Kumar and B. Bandyopadhyay, *J. Phys. Chem. A*, 2018, **122**, 350-363.)

Table S4 Equilibrium constants (cm^3·molecule^{-1}) for three-body complexes constituted by H_2O_2, HO and catalyst X (X = NH_3 and HCOOH) within the temperature range of 213-320 K

T/K	K_{eq}(R1)	K_{eq}(R_WM)	K_{eq}(R_AM1)	K_{eq}(R_AM2a)	K_{eq}(R_AM2b)	K_{eq}(R_AM3a)	K_{eq}(R_AM3b)	K_{eq}(R_FA1)	K_{eq}(R_FA2a)	K_{eq}(R_FA2b)	K_{eq}(R_FA3a)	K_{eq}(R_FA3b)
213	1.46×10^{-11}	2.47×10^{-24}	2.20×10^{-17}	8.20×10^{-28}	1.60×10^{-21}	1.05×10^{-23}	3.33×10^{-15}	2.49×10^{-21}	1.28×10^{-21}	4.40×10^{-15}	3.57×10^{-23}	1.55×10^{-14}
230	1.44×10^{-12}	1.77×10^{-24}	5.80×10^{-18}	1.06×10^{-27}	7.20×10^{-22}	7.95×10^{-24}	4.73×10^{-16}	4.50×10^{-20}	7.80×10^{-22}	6.40×10^{-16}	2.96×10^{-23}	2.14×10^{-15}
259	5.55×10^{-14}	1.09×10^{-24}	9.05×10^{-19}	1.50×10^{-27}	2.40×10^{-22}	5.40×10^{-24}	3.09×10^{-17}	1.09×10^{-20}	3.93×10^{-22}	4.42×10^{-17}	2.34×10^{-23}	1.36×10^{-16}
280	8.05×10^{-15}	8.10×10^{-25}	3.01×10^{-19}	1.84×10^{-27}	1.26×10^{-22}	4.33×10^{-24}	6.15×10^{-18}	4.70×10^{-21}	2.64×10^{-22}	9.10×10^{-18}	2.06×10^{-23}	2.67×10^{-17}
290	3.54×10^{-15}	7.15×10^{-25}	1.89×10^{-19}	2.00×10^{-27}	9.65×10^{-23}	3.94×10^{-24}	3.10×10^{-18}	3.30×10^{-21}	2.24×10^{-22}	4.68×10^{-18}	1.96×10^{-23}	1.35×10^{-17}
298	1.91×10^{-15}	6.50×10^{-25}	1.33×10^{-19}	2.13×10^{-27}	7.90×10^{-23}	3.68×10^{-24}	1.86×10^{-18}	2.53×10^{-21}	1.98×10^{-22}	2.84×10^{-18}	1.89×10^{-23}	8.05×10^{-18}
300	1.65×10^{-15}	6.35×10^{-25}	1.22×10^{-19}	2.16×10^{-27}	7.50×10^{-23}	3.62×10^{-24}	1.64×10^{-18}	2.38×10^{-21}	1.92×10^{-22}	2.52×10^{-18}	1.87×10^{-23}	7.10×10^{-18}
310	8.05×10^{-16}	5.70×10^{-25}	8.15×10^{-20}	2.32×10^{-27}	5.95×10^{-23}	3.34×10^{-24}	9.05×10^{-19}	1.75×10^{-21}	1.67×10^{-22}	1.41×10^{-18}	1.80×10^{-23}	3.92×10^{-18}
320	4.11×10^{-16}	5.10×10^{-25}	5.60×10^{-20}	2.48×10^{-27}	4.81×10^{-23}	3.10×10^{-24}	5.20×10^{-19}	1.32×10^{-21}	1.47×10^{-22}	8.20×10^{-19}	1.74×10^{-23}	2.25×10^{-18}

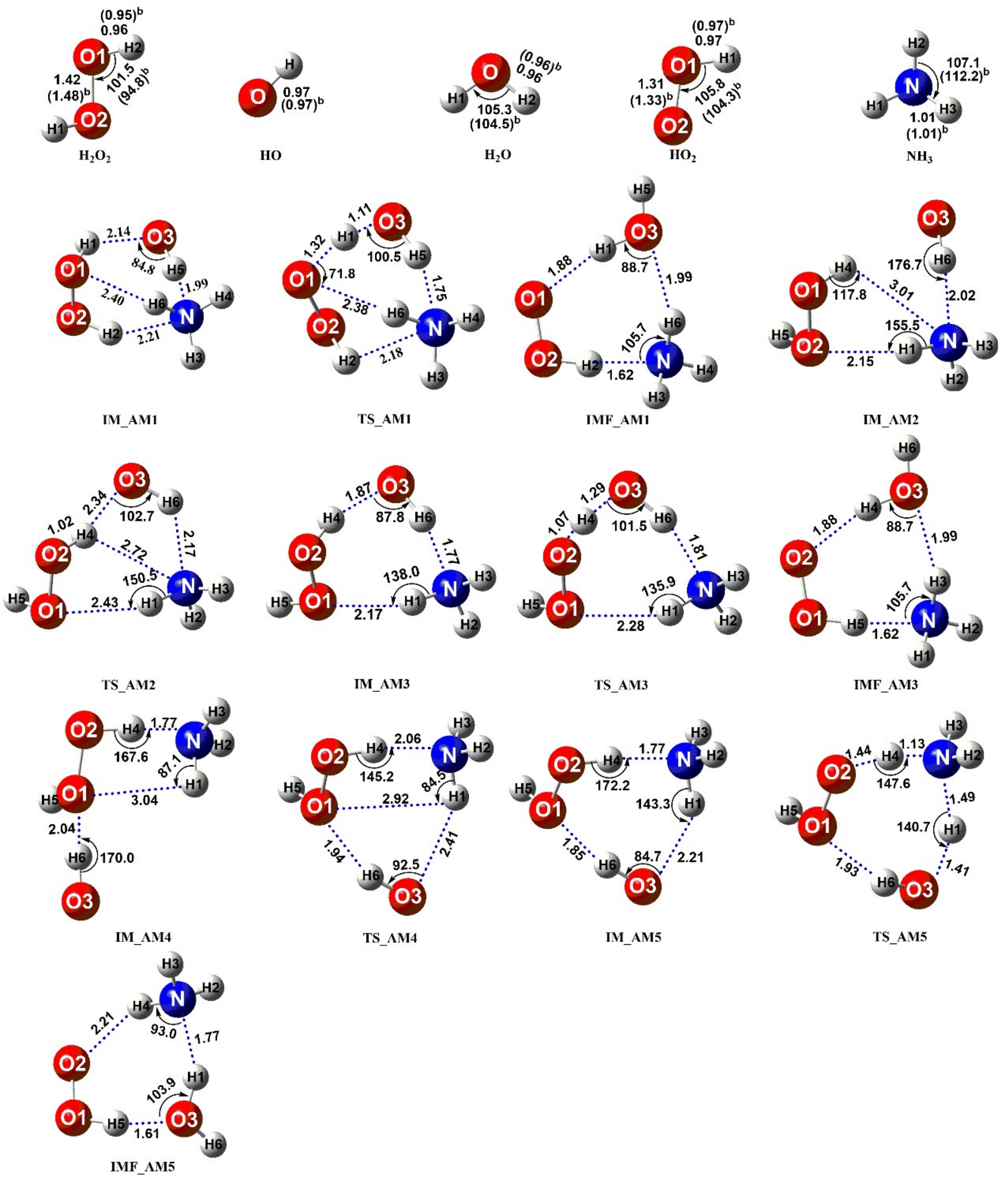


Fig. S4 Optimized geometries for NH_3 catalyzed H_2O_2 + HO → HO_2 + H_2O reaction at the M06-2X/aug-cc-pVTZ level

^{b} Value was from the NIST chemistry Webbook (http://webbook.nist.gov/ chemistry.)

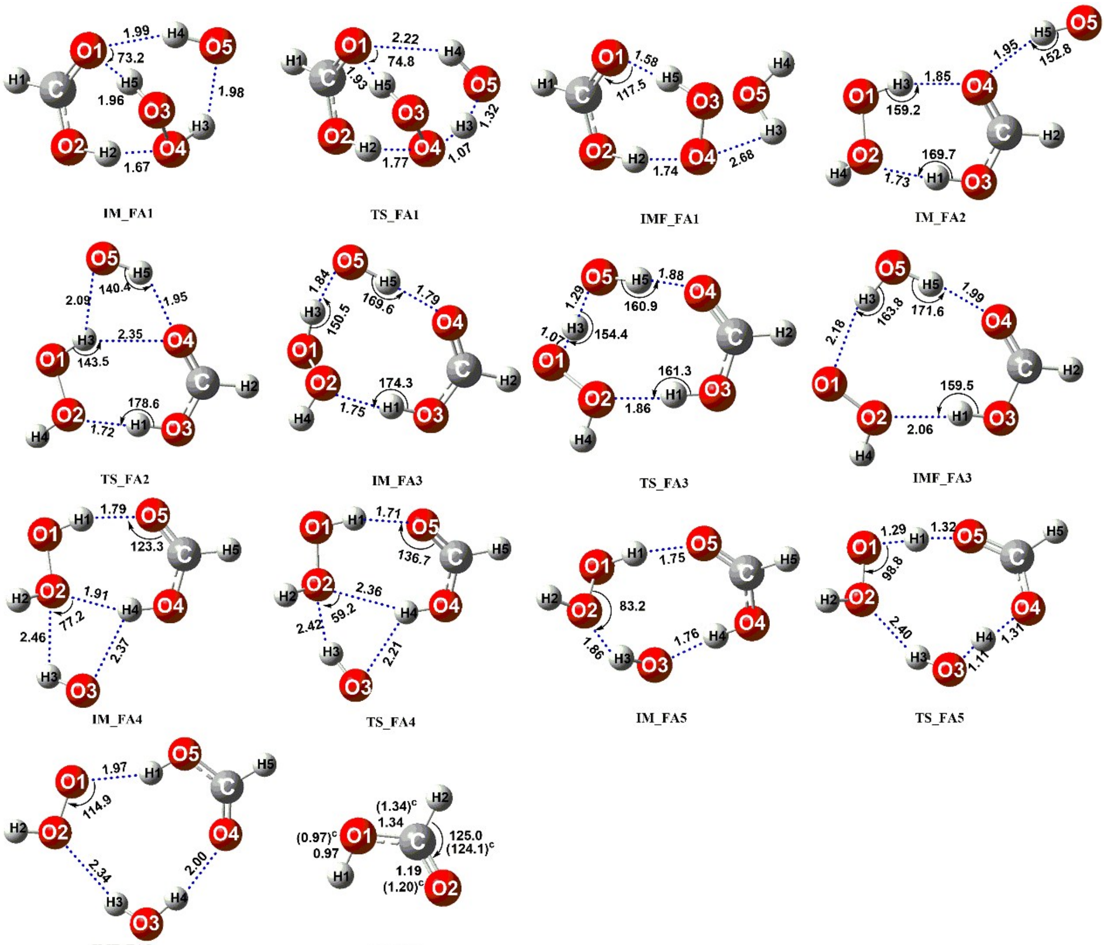


Fig. S5 Optimized geometries for HCOOH catalyzed $H_2O_2 + HO \rightarrow HO_2 + H_2O$ reaction at the M06-2X/aug-cc-pVTZ level

[c] Value was from the NIST chemistry Webbook (http://webbook.nist.gov/chemistry.)

Table S5 Relative energies ((ΔE), (ΔE + ZPE)), enthalpies (ΔH), and free energies for the reactants, intermediate, and transition states involved in the H_2O_2 + HO → HO_2 + H_2O reaction with catalyst *X* (*X* = NH_3 and HCOOH) at the CCSD(T)-F12a/cc-pVDZ-F12//M06-2X/ aug-cc-pVTZ level

Species	ΔE(298) (kcal·mol^{-1})	ΔH(298) (kcal·mol^{-1})	ΔG(298) (kcal·mol^{-1})	$\Delta(E$ + ZPE)(298) (kcal·mol^{-1})
H_2O_2 + HO	0.0	0.0	0.0	0.0
IM1	-13.7	-12.5	-5.1	-11.8
TS1	2.6	0.9	9.0	2.3
IMF1	-35.4	-33.5	-28.2	-33.4
H_2O + HO_2	-32.0	-31.7	-32.9	-31.7
H_2O_2 + H_2O + HO	0.0	0.0	0.0	0.0
$H_2O_2\cdots H_2O$ + HO	-7.1	-5.3	3.1	-4.7
IM_WM	-12.5	-9.5	7.0	-8.5
TS_WM	-6.4	-6.3	12.0	-4.5
IMF_WM	-52.7	-48.9	-31.0	-47.4
$2H_2O$ + HO_2	-32.0	-31.7	-32.9	-31.7
H_2O_2 + NH_3 + HO	0.0	0.0	0.0	0.0
$H_2O_2\cdots NH_3$ + HO	-8.6	-6.9	0.8	-6.6
IM_AM1	-20.1	-17.1	-1.0	-16.1
TS_AM1	-8.7	-8.3	8.6	-6.9
IMF_AM1	-53.8	-50.2	-33.2	-49.1
H_2O + HO_2 + NH_3	-32.0	-31.7	-32.9	-31.7
H_2O_2 + NH_3 + HO	0.0	0.0	0.0	0.0
$H_2O_2\cdots NH_3$ + HO	-8.6	-6.9	0.8	-6.6
$HO\cdots NH_3$ + H_2O_2	-7.8	-6.3	1.1	-5.5
IM_AM2	-10.5	-8.3	9.7	-6.5
TS_AM2	-7.2	-5.5	12.0	-3.9
IM_AM3	-16.4	-12.9	4.2	-11.8
TS_AM3	-8.2	-9.0	8.6	-7.4
IMF_AM3	-53.8	-50.2	-33.1	-49.1
H_2O + HO_2 + NH_3	-32.0	-31.7	-32.9	-31.7
H_2O_2 + NH_3 + HO	0.0	0.0	0.0	0.0
$H_2O_2\cdots NH_3$ + HO	-8.6	-6.9	0.8	-6.6
$NH_3\cdots HO$ + H_2O_2	-1.6	-0.4	6.2	0.0
IM_AM4	-13.5	-10.9	5.5	-9.8
TS_AM4	-8.0	-6.2	11.4	-4.6
IM_AM5	-17.4	-14.4	2.5	-13.3
TS_AM5	21.1	19.6	39.8	22.1
IMF_AM5	-53.0	-49.4	-31.9	-48.2
H_2O + HO_2 + NH_3	-32.0	-31.7	-32.9	-31.7
H_2O_2 + HCOOH + HO	0.0	0.0	0.0	0.0
$H_2O_2\cdots$HCOOH + HO	-12.1	-10.5	-0.5	-10.1
IM_FA1	-19.5	-16.8	1.6	-16.0
TS_FA1	-10.7	-11.0	8.8	-9.5
IMF_FA1	-50.8	-47.7	-29.8	-47.3
H_2O + HO_2 + HCOOH	-32.0	-31.7	-32.9	-31.7
H_2O_2 + HCOOH + HO	0.0	0.0	0.0	0.0
$H_2O_2\cdots$HCOOH + HO	-12.1	-10.5	-0.5	-10.1
$HO\cdots$HCOOH + H_2O_2	-5.5	-4.1	4.4	-4.9
IM_FA2	-18.3	-15.3	2.0	-14.7
TS_FA2	-14.2	-12.3	6.2	-11.3
IM_FA3	-19.8	-16.9	1.3	-16.2
TS_FA3	-7.9	-8.6	10.2	-7.3

IMF_FA3	-40.9	-37.7	-22.8	-37.5
$H_2O + HO_2 + HCOOH$	-32.0	-31.7	-32.9	-31.7
$H_2O_2 + HCOOH + HO$	0.0	0.0	0.0	0.0
$H_2O_2 \cdots HCOOH + HO$	-12.1	-10.5	-0.5	-10.1
$HO \cdots HCOOH + H_2O_2$	-5.5	-4.1	4.4	-4.9
IM_FA4	-15.7	-13.0	4.2	-12.6
TS_FA4	-12.6	-10.4	8.5	-9.2
IM_FA5	-19.9	-17.1	0.8	-16.4
TS_FA5	19.6	16.1	37.2	18.4
IMF_FA5	-42.6	-39.6	-23.1	-39.4
$H_2O + HO_2 + HCOOH$	-32.0	-31.7	-32.9	-31.7

Table S6 Calculated rate coefficients (cm^3·molecules^{-1}·s^{-1}) for the H_2O_2 + HO → HO_2 + H_2O reaction in the presence of catalyst *X* (*X* = NH_3 and HCOOH) within the temperature range of 213-320 K

T/K	$k_{\mathrm{R\_WM}}$	$k_{\mathrm{R\_AM1}}$	$k_{\mathrm{R\_AM2a}}$	$k_{\mathrm{R\_AM2b}}$	$k_{\mathrm{R\_AM3a}}$	$k_{\mathrm{R\_AM3b}}$
213	9.46×10^{-12}	1.11×10^{-9}	2.71×10^{-17}	5.72×10^{-10}	5.13×10^{-36}	1.63×10^{-27}
230	8.48×10^{-12}	5.31×10^{-10}	5.13×10^{-17}	2.78×10^{-10}	1.20×10^{-35}	7.13×10^{-28}
259	7.34×10^{-12}	2.15×10^{-10}	1.23×10^{-16}	1.04×10^{-10}	6.34×10^{-35}	3.63×10^{-28}
280	6.82×10^{-12}	1.35×10^{-10}	2.06×10^{-16}	5.91×10^{-11}	2.49×10^{-34}	3.54×10^{-28}
290	6.65×10^{-12}	1.13×10^{-10}	2.54×10^{-16}	4.68×10^{-11}	4.98×10^{-34}	3.92×10^{-28}
298	6.53×10^{-12}	9.95×10^{-11}	2.98×10^{-16}	3.93×10^{-11}	8.84×10^{-34}	4.47×10^{-28}
300	6.51×10^{-12}	9.64×10^{-11}	3.09×10^{-16}	3.75×10^{-11}	1.02×10^{-33}	4.63×10^{-28}
310	6.41×10^{-12}	8.39×10^{-11}	3.70×10^{-16}	3.06×10^{-11}	2.14×10^{-33}	5.81×10^{-28}
320	6.27×10^{-12}	7.43×10^{-11}	4.38×10^{-16}	2.55×10^{-11}	4.58×10^{-33}	7.69×10^{-28}

T/K	$k_{\mathrm{R\_FA1}}$	$k_{\mathrm{R\_FA2a}}$	$k_{\mathrm{R\_FA2b}}$	$k_{\mathrm{R\_FA3a}}$	$k_{\mathrm{R\_FA3b}}$
213	2.50×10^{-11}	5.90×10^{-13}	3.58×10^{-6}	6.11×10^{-32}	2.65×10^{-23}
230	5.48×10^{-10}	5.10×10^{-13}	6.64×10^{-7}	1.14×10^{-31}	8.24×10^{-24}
259	1.80×10^{-10}	4.27×10^{-13}	6.84×10^{-8}	3.92×10^{-31}	2.28×10^{-24}
280	9.50×10^{-11}	3.95×10^{-13}	1.86×10^{-8}	1.07×10^{-30}	1.38×10^{-24}
290	7.32×10^{-11}	3.87×10^{-13}	1.09×10^{-8}	1.78×10^{-30}	1.22×10^{-24}
298	6.07×10^{-11}	3.82×10^{-13}	7.29×10^{-9}	2.70×10^{-30}	1.15×10^{-24}
300	5.81×10^{-11}	3.81×10^{-13}	6.64×10^{-9}	3.00×10^{-30}	1.14×10^{-24}
310	4.67×10^{-11}	3.78×10^{-13}	4.20×10^{-9}	5.17×10^{-30}	1.13×10^{-24}
320	3.83×10^{-11}	3.79×10^{-13}	2.76×10^{-9}	9.05×10^{-30}	1.17×10^{-24}

Table S7 Effective rate coefficients (k_t') (cm^3·molecules^{-1}·s^{-1}) for the H_2O_2 + HO → HO_2 + H_2O reaction with basic (NH_3) and acidic (HCOOH) within the temperature range of 280-320 K

T/K	k_t'(R_AM1) (10 ppbv)	k_t'(R_AM1) (2900 ppbv)	k_t'(R_AM2a) (10 ppbv)	k_t'(R_AM2a) (2900 ppbv)	k_t'(R_AM2b) (10 ppbv)	k_t'(R_AM2b) (2900 ppbv)	k_t'(R_AM3a) (10 ppbv)	k_t'(R_AM3a) (2900 ppbv)	k_t'(R_AM3b) (10 ppbv)	k_t'(R_AM3b) (2900 ppbv)
280	5.25×10^{-20}	1.53×10^{-17}	7.97×10^{-26}	2.33×10^{-23}	1.33×10^{-20}	3.88×10^{-18}	9.65×10^{-44}	2.82×10^{-41}	2.80×10^{-41}	8.18×10^{-39}
290	3.20×10^{-20}	9.35×10^{-18}	7.18×10^{-26}	2.10×10^{-23}	8.18×10^{-21}	2.39×10^{-18}	1.41×10^{-43}	4.11×10^{-41}	3.32×10^{-41}	9.70×10^{-39}
298	2.29×10^{-20}	6.50×10^{-18}	6.85×10^{-26}	1.95×10^{-23}	5.84×10^{-21}	1.66×10^{-18}	2.03×10^{-43}	5.77×10^{-41}	4.12×10^{-41}	1.17×10^{-38}
300	2.02×10^{-20}	5.99×10^{-18}	6.49×10^{-26}	1.92×10^{-23}	5.18×10^{-21}	1.53×10^{-18}	2.15×10^{-43}	6.35×10^{-41}	4.18×10^{-41}	1.24×10^{-38}
310	1.39×10^{-20}	3.99×10^{-18}	6.13×10^{-26}	1.76×10^{-23}	3.52×10^{-21}	1.01×10^{-18}	3.55×10^{-43}	1.02×10^{-40}	5.78×10^{-41}	1.66×10^{-38}
320	9.49×10^{-21}	2.76×10^{-1}8	5.59×10^{-26}	1.63×10^{-23}	2.37×10^{-21}	6.90×10^{-19}	5.85×10^{-43}	1.70×10^{-40}	8.08×10^{-41}	2.35×10^{-38}

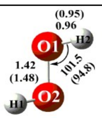
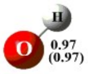
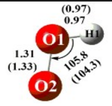
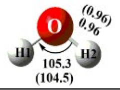
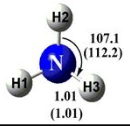
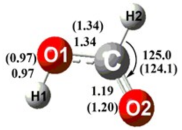
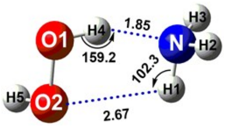
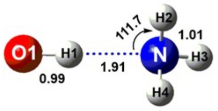
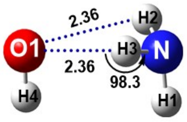
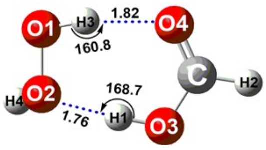
T/K	k_t'(R_FA1) (Low,0.01 ppbv)	k_t'(R_FA1) (High,10 ppbv)	k_t'(R_FA2a) (Low,0.01 ppbv)	k_t'(R_FA2a) (High,10 ppbv)	k_t'(R_FA2b) (Low,0.01 ppbv)	k_t'(R_FA2b) (High,10 ppbv)	k_t'(R_FA3a) (Low,0.01 ppbv)	k_t'(R_FA3a) (High,10 ppbv)	k_t'(R_FA3b) (Low,0.01 ppbv)	k_t'(R_FA3b) (High,10 ppbv)
280	5.19×10^{-22}	5.19×10^{-19}	2.16×10-^{24}	2.16×10^{-21}	9.90×10^{-23}	9.90×10^{-20}	5.83×10^{-42}	5.83×10^{-39}	7.38×10^{-39}	7.38×10^{-36}
290	2.34×10^{-22}	2.34×10^{-19}	1.24×10^{-24}	1.24×10^{-21}	5.05×10^{-23}	5.05×10^{-20}	5.68×10^{-42}	5.68×10^{-39}	5.69×10^{-39}	5.69×10^{-36}
298	1.27×10^{-22}	1.27×10^{-19}	8.03×10^{-25}	8.03×10^{-22}	3.05×10^{-23}	3.05×10^{-20}	5.67×10^{-42}	5.67×10^{-39}	4.80×10^{-39}	4.80×10^{-36}
300	1.12×10^{-22}	1.12×10^{-19}	7.31×10^{-25}	7.31×10^{-22}	2.72×10^{-23}	2.72×10^{-20}	5.76×10^{-42}	5.76×10^{-3}9	4.67×10^{-39}	4.67×10^{-36}
310	5.82×10^{-23}	5.82×10^{-20}	4.72×10^{-25}	4.72×10^{-22}	1.59×10^{-23}	1.59×10^{-20}	6.45×10^{-42}	6.45×10^{-39}	4.27×10^{-39}	4.27×10^{-36}
320	3.07×10^{-23}	3.07×10^{-20}	3.04×10^{-25}	3.04×10^{-22}	9.33×10^{-24}	9.33×10^{-21}	7.26×10^{-42}	7.26×10^{-39}	3.96×10^{-39}	3.96×10^{-36}

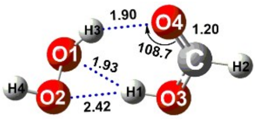
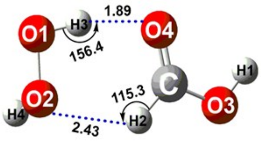
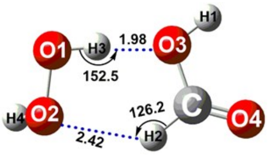
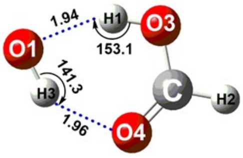
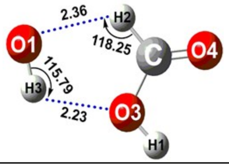
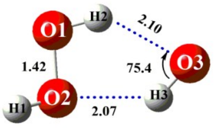
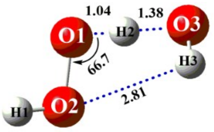
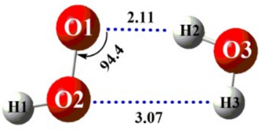
Table S8 Concentrations of *X* (*X* = H_2O, NH_3, HCOOH and H_2SO_4) (in molecule·cm^{-3}) within the temperature range of 280-320 K at 0 km altitude

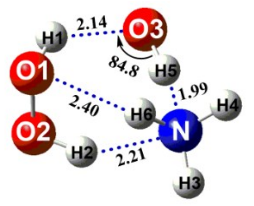
Catalyst		280 K	290 K	298 K	300 K	310 K	320 K
H_2O	20% RH	5.2×10^{16}	9.6×10^{16}	1.5×10^{17}	1.7×10^{17}	2.9×10^{17}	4.1×10^{17}
	40% RH	1.0×10^{17}	1.9×10^{17}	3.1×10^{17}	3.4×10^{17}	5.8×10^{17}	9.4×10^{17}
	60% RH	1.5×10^{17}	2.9×10^{17}	4.5×10^{17}	5.1×10^{17}	8.8×10^{17}	1.4×10^{17}
	80% RH	2.1×10^{17}	3.8×10^{17}	6.2×10^{17}	6.9×10^{17}	1.2×10^{17}	1.9×10^{17}
	100% RH	2.6×10^{17}	4.8×10^{17}	7.7×10^{17}	8.6×10^{17}	1.5×10^{18}	2.3×10^{18}
NH_3	0.1 ppbv	2.6×10^{9}	2.5×10^{9}	2.5×10^{9}	2.4×10^{9}	2.4×10^{9}	2.3×10^{9}
	10 ppbv	2.6×10^{11}	2.5×10^{11}	2.5×10^{11}	2.4×10^{11}	2.4×10^{11}	2.3×10^{11}
	2900 ppbv	7.6×10^{13}	7.3×10^{13}	7.1×10^{13}	7.1×10^{13}	6.9×10^{13}	6.7×10^{13}
HCOOH	High	2.6×10^{11}	2.5×10^{11}	2.4×10^{11}	2.4×10^{11}	2.4×10^{11}	2.3×10^{11}
	Average	2.0×10^{10}	1.9×10^{10}	1.9×10^{10}	1.9×10^{10}	1.8×10^{10}	1.8×10^{10}
	Low	2.6×10^{8}	2.5×10^{8}	2.4×10^{8}	2.4×10^{8}	2.4×10^{8}	2.3×10^{8}
H_2SO_4		3.9×10^{8}	3.8×10^{8}	3.7×10^{8}	3.7×10^{8}	3.6×10^{8}	3.4×10^{8}

The Value was from Ref (S. Sarkar, S. Mallick, Deepak, P. Kumar and B. Bandyopadhyay, *Phys. Chem. Chem. Phys.*, 2017, **19**, 27848-27858.)

Table S9 Coordinates and geometrical structures for the reactants, pre-reactive complexes, transition states, post-reactive complexes and products involved in catalyst *X* (*X* = NH_3 and HCOOH) assisted $H_2O_2 + HO \rightarrow HO_2 + H_2O$ reaction at the M06-2X/aug-cc-pVTZ level

Coordinate	**Frequency**	**Structure**
H_2O_2		
O 0.00000000 0.71154400 -0.05812700 H 0.78644300 0.90348800 0.46501400 O 0.00000000 -0.71154400 -0.05812700 H -0.78644300 -0.90348800 0.46501400	373.20 1044.11 1355.52 1464.95 3837.21 3838.44	
HO		
O 0.00000000 0.00000000 0.10799800 H 0.00000000 0.76273400 -0.86398300	3744.37	
HO_2		
O 0.05507400 -0.60010800 0.00000000 H -0.88118600 -0.86505400 0.00000000 O 0.05507400 0.70824000 0.00000000	1225.01 1462.80 3690.48	
H_2O		
O 0.00000000 0.00000000 0.11635900 H 0.00000000 0.76273400 -0.46543500 H 0.00000000 -0.76273400 -0.46543500	1616.15 3871.58 3975.57	
NH_3		
N 0.00002600 0.00002600 -0.11246200 H -0.56199200 0.75354600 0.26242100 H 0.93368900 0.10967600 0.26246600 H -0.37188100 -0.86340400 0.26234800	1034.34 1660.37 1661.74 3508.74 3631.81 3638.12	
HCOOH		
C 0.13498200 0.39878300 -0.00000100 H 0.11130600 1.49338900 0.00002400 O 1.12637700 -0.26486600 -0.00007800 O -1.11039500 -0.08900800 0.00007000 H -1.04905500 -1.05509200 0.00004600	645.75 676.77 1074.92 1159.99 1317.64 1409.70 1869.19 3120.09 3791.33	
$H_2O_2 \cdots NH_3$		
O 0.88714900 0.77306500 0.00826100 O 1.22938000 -0.60714700 -0.11079000 H -0.09051100 0.69895200 0.08496800 H 1.70982200 -0.75728200 0.70975400 N -1.77359500 -0.05618800 0.02027800 H -1.41706300 -0.96824900 -0.24227100 H -2.37903000 0.26444400 -0.72444600 H -2.34029500 -0.17188800 0.85028200	60.38 96.86 207.80 238.24 304.88 366.07 805.77 1037.65 1083.02 1373.96 1575.41 1654.79 1659.96 3419.71 3498.60 3617.01 3632.93 3847.12	
$HO \cdots NH_3$		
O -1.63607200 0.00002000 0.00000500 H -0.64793100 0.00074400 0.00002700 N 1.26201500 0.00029000 0.00000700 H 1.63291400 -0.48603000 -0.80700100 H 1.63324700 -0.45789900 0.82315100 H 1.63624200 0.94099400 -0.01626700	205.86 215.26 227.96 609.57 746.91 1101.28 1657.89 1658.23 3421.11 3501.26 3621.82 3624.48	
$NH_3 \cdots HO$		
O -1.37047200 -0.09049300 -0.00000200 H -1.34904800 0.88052400 0.00022400 N 1.32844400 -0.05387500 -0.00007700 H 0.82538600 -0.36848200 0.81946100 H 0.82493000 -0.36729500 -0.81978900 H 1.36339500 0.95632100 0.00065300	129.12 161.62 263.61 319.84 373.93 963.28 1644.35 1652.56 3506.10 3638.91 3650.31 3756.60	
$H_2O_2 \cdots HCOOH$		
O 1.55584000 0.69661000 0.13281900 O 1.73992300 -0.65781100 -0.26179400 H 0.84669000 -1.02544900 -0.09887800 C -1.61073800 -0.12441600 0.00431400 H -2.70341600 -0.14075900 -0.04153800 O -0.94617700 -1.11693300 0.17563100 O -1.13719200 1.09317100 -0.14785100 H -0.15362300 1.07050600 -0.07639500 H 1.97562300 0.72189500 1.00048500	75.77 162.03 189.64 208.41 254.68 357.11 682.05 706.19 910.57 1043.44 1095.07 1252.68 1369.79 1400.60 1435.54 1555.16 1808.67 3135.61 3379.09 3545.07 3821.65	
$H_2O_2 \cdots HCOOHa$		

O	1.38408000	0.13909100	0.69856100				
O	1.87547100	-0.17417000	-0.60242900	73.57	115.92	163.43	
H	2.76075400	0.20609600	-0.57514200	193.82	222.96	261.49	
C	-1.60883100	0.05130400	-0.17420800	685.93	731.48	827.12	
H	-2.63246700	-0.06303800	-0.54329200	1042.81	1086.99	1230.54	
O	-1.06660400	1.12035300	-0.05227700	1381.43	1435.73	1501.96	
O	-1.07371900	-1.12175300	0.11180400	1820.45	3126.70	3544.13	
H	-0.15486200	-0.99140400	0.42294600	3608.98	3836.78		
H	0.72574500	0.83235900	0.49545500				
H_2O_2···HCOOHb							
O	-1.86089400	-0.81414000	0.11985700				
O	-2.04315800	0.53933900	-0.28694400	48.59	70.13	130.07	
H	-1.17878700	0.91765500	-0.04818100	142.82	212.37	261.94	
C	1.11575900	-0.14804700	-0.08924200	646.04	663.01	688.14	
H	0.49652700	-0.98233300	-0.42710800	1040.96	1094.6	1180.61	
O	0.68405200	0.91828500	0.25856300	1333.58	1377.9	1419.56	
O	2.40845400	-0.45580700	-0.10303800	1523.22	1827.7	3163.83	
H	2.90660100	0.31543100	0.20517500	3648.86	3782.81	3847.92	
H	-2.42652700	-0.86388600	0.89805400				
H_2O_2···HCOOHc							
O	-1.84107100	-0.81775500	0.13133900				
O	-2.09715500	0.51458100	-0.30052100	49.84	60.64	115.26	
H	-1.25012200	0.93851800	-0.09870900	125.07	176.00	249.22	
C	1.29461400	-0.28553000	-0.08176200	534.54	646.88	655.63	
H	0.52958500	-1.03873600	-0.28846900	1043.31	1083.28	1138.60	
O	2.47410200	-0.44608000	-0.10402200	1290.81	1376.40	1427.71	
O	0.70794300	0.89417600	0.21966100	1501.95	1880.10	3156.23	
H	1.40843900	1.53851400	0.39701900	3741.16	3792.45	3841.16	
H	-2.40613600	-0.88449900	0.90907300				
HO···HCOOH							
O	-2.02456300	0.04344200	-0.00003400				
H	-1.40220800	-0.71874400	-0.00004600	182.23	182.57	205.68	
C	1.13252600	-0.09467000	-0.00005400	445.07	647.36	700.04	
H	2.22563700	-0.05031300	-0.00025100	762.13	1086.47	1228.71	
O	0.51081400	-1.12601500	0.00005800	1384.69	1431.16	1821.95	
O	0.60754600	1.11894800	0.00003000	3130.91	3531.54	3591.88	
H	-0.36896200	1.04608200	0.00018400				
HO···HCOOHa							
O	2.56597000	-0.27267900	-0.00002600				
H	1.81621500	0.35782000	0.00005300	41.85	71.59	189.22	
C	-0.63058700	-0.22076600	0.00003800	431.42	589.70	663.21	
H	-0.12953300	-1.19357300	0.00011700	684.12	1082.41	1185.49	
O	-0.05894300	0.83487300	0.00001300	1340.05	1425.50	1838.13	
O	-1.95125100	-0.35779600	-0.00002600	3154.91	3610.23	3771.31	
H	-2.34935700	0.52516300	-0.00009100				
IM1							
O	-0.95522900	-0.73526400	0.01828600				
H	-0.02774900	-0.97402600	-0.13811700	179.12	196.21	223.65	
O	-0.86558300	0.68416000	0.09032400	274.29	432.39	566.24	
O	1.84145000	-0.02945500	-0.03015800	1040.23	1369.77	1512.90	
H	-1.33684200	0.95242300	-0.70684500	3642.06	3728.66	3831.80	
H	1.19948700	0.66607000	0.21734600				
TS1							
O	-1.24106100	-0.45309600	-0.14211000				
H	-1.62022800	-0.60532400	0.73199600	-1493.30	135.36	238.40	
O	-0.48707800	0.70571500	0.06782000	362.52	404.19	688.58	
O	1.68977700	-0.11037900	-0.02767000	1068.87	1366.07	1518.61	
H	0.45016300	0.43890100	-0.28222200	1820.29	3778.57	3828.05	
H	1.47695900	-0.97149700	0.36590600				
IMF1							
O	1.20764500	-0.55952100	0.00291800				
H	2.17920000	-0.61549000	0.02280300	43.10	119.05	151.14	
O	0.92203300	0.71591900	-0.00671400	158.58	272.84	410.06	
O	-2.02690500	-0.01271000	0.00965200	1259.89	1457.48	1643.40	
H	-1.16455000	0.41516100	0.00030700	3669.96	3834.54	3953.88	
H	-1.83683400	-0.94917300	-0.06995700				
IM_AM1							

O	1.24635200	0.48811400	-0.70117900				
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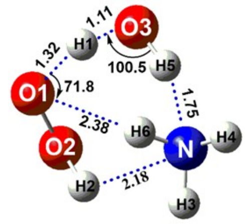
O	-0.88705500	-0.89193200	-0.52434700				
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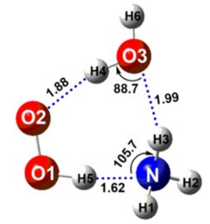
O	-1.64897900	0.02409200	0.02121800				
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H	2.29633200	-1.63438500	0.11558800	1187.41	1316.61	1632.26	
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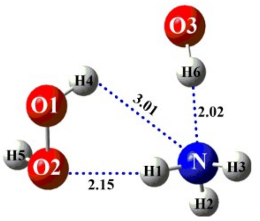
N	1.00904500	1.44344100	-0.17217000				
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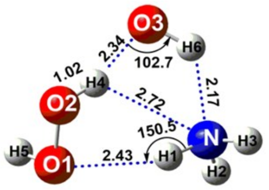
N	1.32621200	1.35207400	-0.09172000				
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O	-1.85365400	0.38700000	0.38658900	1561.74	1663.82	1670.36	
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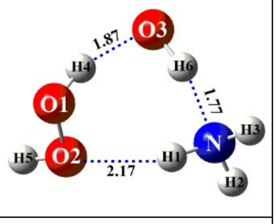
O	-1.38184800	0.12501100	0.66515600				
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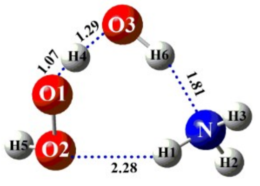
O	-1.26627500	0.06992800	0.59502400				
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H	1.08940400	-1.21135900	-0.06543300	1084.58	1110.08	1288.73	
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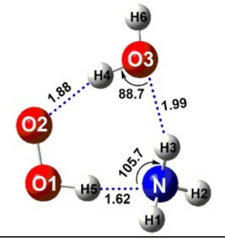
O	1.78508000	-0.83386600	-0.00776700				
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O	-1.03811700	-1.12637700	-0.02159500	344.92	349.63	403.20	
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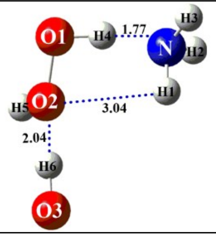
O	0.92862500	-1.34090100	-0.23364700				
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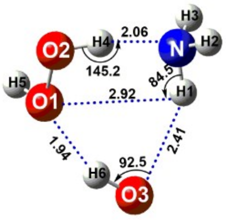
O	-1.77760200	-0.42289000	-0.08748000				
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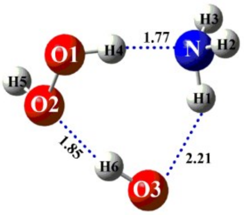
N	1.25650800	-1.37014100	0.10449500				
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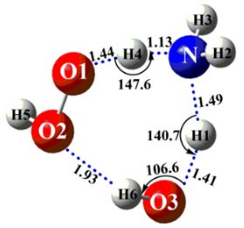
N	1.38678000	-0.97400100	0.11261500				
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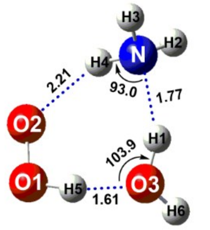
N	1.38678000	-0.97400100	0.11261500				
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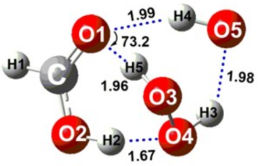
O	0.98457400	-1.15247200	-0.48798900	62.54	103.93	135.85	
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H	-0.66248700	-0.95449400	-0.67310400	1780.66	3119.42	3152.72	
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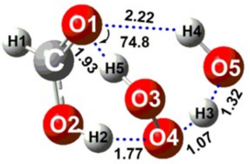
O	-1.23543600	0.58199900	-0.64650400				
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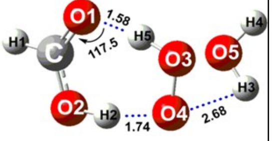
O	1.42386100	-0.78711200	-0.72364600				
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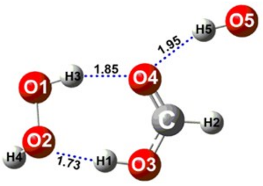
O	2.40585100	-0.03204800	0.20506300				
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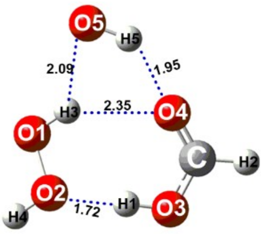
O	0.25353100	1.87980100	0.20203500				
O	1.38119700	1.21452400	-0.35346000	-66.64	52.19	74.04	
H	1.19362800	0.27576900	-0.15056200	145.85	152.47	191.29	
C	-1.66430300	-0.88008500	-0.03840500	197.68	225.09	296.82	
H	-2.53237600	-1.53938400	-0.13086700	333.34	516.00	563.44	
O	-0.53377300	-1.29065000	0.09812500	698.24	930.82	1045.76	
O	-2.00246000	0.38689100	-0.09172300	1092.63	1261.64	1378.75	
H	-1.19033900	0.94196700	0.00988700	1401.11	1434.08	1465.46	
H	0.59584900	2.21545300	1.04051800	1792.28	3143.58	3346.54	
O	2.22674700	-1.53078900	0.06640900	3635.93	3652.60	3822.58	
H	1.31711200	-1.89152500	0.09036900				
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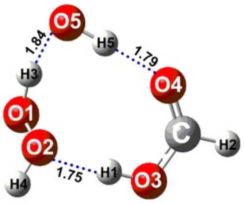
O	-1.12029800	-1.05448000	0.56600600				
O	-1.63026800	-0.78236600	-0.73510100	52.82	67.33	91.29	
H	-1.78059500	0.18131400	-0.65199100	114.16	195.25	197.90	
C	1.93962900	0.14854200	-0.11452900	223.46	250.78	315.08	
H	3.00581100	0.20875600	-0.35354300	481.94	572.55	686.66	
O	1.23919100	1.12570000	-0.01809800	809.59	888.41	1045.43	
O	1.55615300	-1.09627700	0.04686100	1094.54	1252.94	1342.43	
H	0.59516700	-1.13928100	0.25548800	1396.49	1433.10	1503.69	
H	-1.79208400	-1.63572300	0.93962700	1813.38	3132.48	3426.31	
O	-1.44425900	1.79040900	0.17840200	3484.66	3569.53	3839.66	
H	-0.47022600	1.62978400	0.19302800				
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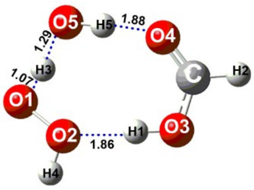
O	-1.15684600	-1.19233300	0.26882200				
O	-2.18793200	-0.27497100	0.07067700	-1967.03	39.26	80.79	
H	-1.70980900	0.54653600	-0.43127800	94.72	151.31	182.66	
C	1.97228600	0.02172800	0.05340400	215.47	243.39	436.81	
H	3.06006500	0.06956300	-0.05269700	458.87	540.58	686.04	
O	1.34735100	0.73745300	0.79636800	839.94	869.65	1080.44	
O	1.45530300	-0.90657600	-0.72490900	1095.19	1234.15	1331.79	
H	0.48778000	-0.95797400	-0.57477600	1382.71	1413.50	1429.46	
H	-1.01218600	-1.15146700	1.22404800	1496.93	1810.95	3140.50	
O	-1.00967500	1.62389300	-0.48509500	3520.11	3585.96	3786.33	
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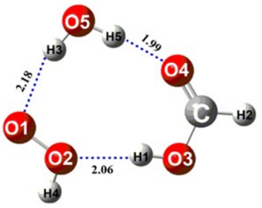
O	-1.47013800	-1.21764300	0.23416900				
O	-2.45186200	-0.41906400	-0.10196200	10.79	47.71	57.67	
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C	2.15213000	-0.20886400	0.01487400	171.35	180.93	251.39	
H	3.22992800	-0.40670100	-0.02479300	367.70	390.09	487.32	
O	1.67007900	0.83984200	0.34631500	662.36	755.09	1085.06	
O	1.45949000	-1.28897000	-0.35027100	1183.74	1249.8	1345.60	
H	0.51018900	-1.07707100	-0.30233900	1425.60	1459.54	1650.24	
H	-1.88172500	-2.01079700	0.62700900	1827.08	3112.57	3635.62	
O	-0.86516300	2.25710400	-0.15775300	3692.63	3802.09	3899.10	
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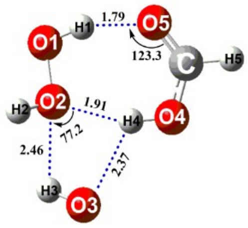
O	-1.07885400	0.84453900	0.25898600				
O	-0.33259600	1.94294600	-0.24956300	35.14	68.10	80.44	
H	0.57742000	1.58563800	-0.18303200	125.00	161.25	184.44	
C	1.80124300	-0.75871200	-0.00580100	198.71	224.42	244.12	
H	2.64856000	-1.45000800	-0.03730300	350.76	377.22	671.08	
O	1.93677900	0.43994700	0.02012300	710.73	867.12	1048.48	
O	0.65833500	-1.40725000	-0.00110300	1094.60	1219.24	1357.01	
H	-0.09365300	-0.77960300	0.05199300	1370.29	1418.87	1548.77	
H	-1.32983500	1.14225700	1.14129600	1811.03	3130.98	3496.48	
O	-2.41966400	-1.23083000	-0.04876200	3560.28	3756.93	3823.49	
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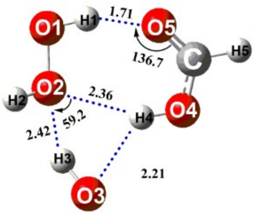
O	-1.34914100	0.86909900	0.08380200				
O	-0.60387500	2.04113300	-0.22455800	-65.45	38.27	101.12	
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C	1.86930700	-0.49182100	0.03279600	190.49	277.29	310.64	
H	2.87705200	-0.91274300	0.05538700	666.72	690.99	781.01	
O	1.64683900	0.68813800	0.16120800	803.35	871.27	1041.14	
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H	0.06317000	-1.00451300	-0.12789600	1381.28	1424.33	1517.56	
H	-1.71253000	1.06111100	0.95684900	1806.17	3159.67	3186.11	
O	-1.98503200	-1.80506200	0.05416800	3522.36	3556.24	3814.82	
H	-2.08154700	-0.90228000	-0.40894000				
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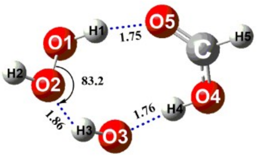
O	1.92026300	-0.32614000	0.71092000				
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C	-1.90973100	-0.50885500	0.10142400	220.48	232.56	255.96	
H	-2.91990200	-0.87189900	0.31397100	458.28	627.41	697.74	
O	-1.00345100	-1.25303100	-0.18597700	735.23	908.00	1037.48	
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H	-0.92884200	1.13151400	0.01425200	1393.85	1425.25	1549.64	
O	0.63293700	1.88832400	-0.27502200	1806.27	3138.62	3331.58	
H	1.32354000	1.34716000	0.16328900	3487.16	3613.52	3854.90	
H	2.66425800	-0.90288000	0.91390600				
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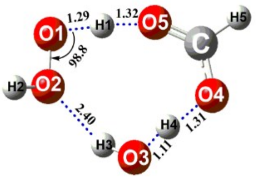
O	-2.00179900	0.39593500	0.03420700				
O	-2.07241200	-0.89611000	0.07974400	-1962.88	-79.16	98.27	
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C	1.67037200	-0.88797600	0.00576000	336.56	384.36	444.36	
H	2.53606100	-1.58201100	0.03511300	510.47	647.78	695.90	
O	0.49527700	-1.30086300	-0.09052600	753.47	1073.56	1157.16	
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O	0.29460100	1.97462600	-0.09425500	1561.71	1683.14	1836.66	
H	-0.29284200	1.94907900	0.67603500	2992.09	3276.32	3780.11	
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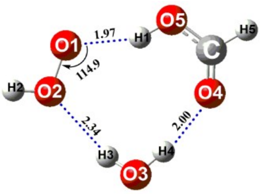
O	2.30091400	-0.30143400	-0.04076500				
O	1.58445900	-1.41690700	-0.04204700	45.91	72.76	87.50	
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C	-2.10393800	-0.35693800	0.02593200	179.42	189.61	210.72	
H	-3.14487400	-0.66888600	0.16622100	312.49	364.35	497.17	
O	-1.29674600	-1.41213800	0.10803700	669.62	805.38	1086.07	
O	-1.76877900	0.78149400	-0.17410300	1185.85	1199.23	1342.49	
H	-0.20146500	2.01011900	0.01304700	1415.32	1453.87	1657.06	
O	0.65826700	2.44037500	0.11952600	1811.61	3126.12	3589.66	
H	1.28423000	1.79559900	-0.22155400	1616.43	1789.37	3912.61	
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