

**Supplementary Information for**  
**H<sub>2</sub>O as a catalyst on the reaction of HONO and**  
**Criegee intermediate (CH<sub>2</sub>OO)**

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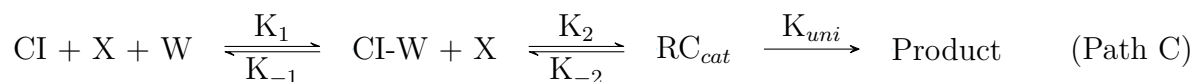
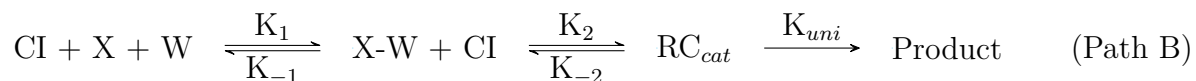
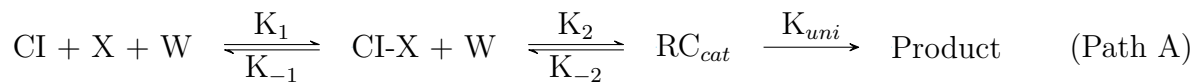
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# 1 Formal proof for same value of termolecular rate constant for path A, B and C



Where CI = CH<sub>2</sub>OO; X = cis-HONO and trans-HONO; W = WM and WD (WM = H<sub>2</sub>O and WD = (H<sub>2</sub>O)<sub>2</sub>).

For path A,

$$K_{eq1} = \frac{[CI - X]}{[CI][X]} \quad (\text{E1})$$

and

$$K_{eq2} = \frac{[RC_{cat}]}{[CI - X][W]} \quad (\text{E2})$$

Therefore,

$$K_{eq1} \times K_{eq2} = \frac{[RC_{cat}]}{[CI][X][W]} \quad (\text{E3})$$

Similarly, for path B,

$$K_{eq1} \times K_{eq2} = \frac{[X - W]}{[X][W]} \times \frac{[RC_{cat}]}{[X - W][CI]} \quad (\text{E4})$$

$$K_{eq1} \times K_{eq2} = \frac{[RC_{cat}]}{[CI][X][W]} \quad (\text{E5})$$

and similarly, for path C,

$$K_{eq1} \times K_{eq2} = \frac{[CI - W]}{[CI][W]} \times \frac{[RC_{cat}]}{[CI - W][X]} \quad (\text{E6})$$

$$K_{eq1} \times K_{eq2} = \frac{[RC_{cat}]}{[CI][X][W]} \quad (\text{E7})$$

From the equation 3, 5 and 7, it is clear that, the product of  $K_{eq1}$  and  $K_{eq2}$  is same for path A, B and C. As the  $k_{uni}$  for path A, B and C are also same, it gives same trimolecular rate  $k_t$ .

Table S1: Optimized geometries in Cartesian coordinates and normal mode frequencies of all species calculate at M062X/aug-cc-pVTZ level of theory

compound	cartesian coordinate(Å)			frequency(cm <sup>-1</sup> )			
CH <sub>2</sub> OO	C	1.057098	-0.186173	-0.000000	538.3305	697.7172	927.1975
	H	1.006168	-1.269153	-0.000000	1023.9710	1260.6781	1433.3721
	H	1.966689	0.398410	-0.000000	1630.8902	3139.9739	3290.5878
	O	0.000000	0.459688	0.000000			
	H	-1.164430	-0.211215	0.000000			
cis-HONO	N	-0.160495	-0.516031	0.000006	686.7057	703.2170	970.3635
	O	1.070217	0.068858	-0.000006	1372.6581	1782.9429	3661.8225
	O	-1.044659	0.253523	-0.000003			
	H	0.918996	1.033168	0.000032			
trans-HONO	N	0.000000	0.507841	-0.000000	578.2458	700.4215	905.0454
	O	-0.882552	-0.567176	0.000000	1342.3941	1841.1078	3830.8277
	O	1.101711	0.141484	-0.000000			
	H	-1.753278	-0.149344	0.000000			
H <sub>2</sub> O	O	-0.000000	0.000000	0.116403	1619.8119	3868.0740	3971.0249
	H	0.000000	0.762572	-0.465611			
	H	-0.000000	-0.762572	-0.465611			
(H <sub>2</sub> O) <sub>2</sub>	O	-1.504794	-0.029013	-0.117920	89.9842	131.5322	141.9149
	O	1.386463	0.023055	0.109603	192.2343	358.2648	611.0779
	H	-1.937073	0.180728	0.711300	1617.8761	1636.3988	3772.6920
	H	-0.556922	0.014790	0.064386	3859.6043	3943.7152	3958.8311
	H	1.725451	0.676007	-0.507602			
	H	1.715190	-0.823861	-0.201556			
Cl-cis-HONO	O	1.036586	-1.124895	0.385188	25.2157	97.1134	104.0131
	O	1.869973	-0.366333	-0.390309	170.0995	200.9472	263.5589
	C	2.060976	0.805543	-0.050328	543.2241	697.1947	740.8312
	H	2.711031	1.380007	-0.698415	890.9788	1001.2501	1024.3023
	H	1.584970	1.187365	0.846651	1090.1125	1266.0754	1450.4279
	N	-2.074269	0.522948	-0.094524	1462.5484	1462.5484	1462.5484
	O	-0.793575	0.738315	0.298145	2987.4652	3134.7497	3281.7521
	O	-2.342006	-0.611644	-0.237751			
	H	-0.309796	-0.144823	0.373216			
Cl-trans-HONO	C	1.422724	1.180300	0.176264	65.1207	91.9279	142.0697
	H	1.037130	1.113235	1.186682	165.9408	223.8118	272.202
	H	1.580393	2.105828	-0.364836	525.7623	695.332	769.4194
	O	1.727404	0.147988	-0.424232	877.0022	1008.9022	1051.5794
	O	1.498260	-1.038558	0.245641	1106.9792	1256.5074	1448.4889
	N	-1.275346	0.258295	0.073862	1556.3251	1678.5345	1793.8428
	O	-1.092608	-1.060602	-0.093796	2996.4334	3141.5958	3286.1768
	O	-2.398526	0.585849	-0.031398			
	H	-0.102689	-1.186339	0.033818			

compound	Cartesian coordinate(Å)			frequency( $\text{cm}^{-1}$ )			
cis-HONO-WM	N	1.358448	0.015234	0.015823	120.5489	146.5676	183.9852
	O	0.585475	-1.079869	0.000804	200.4508	268.5492	405.7981
	O	0.759884	1.035792	0.000334	748.907	884.0683	1061.2885
	H	-0.362567	-0.793271	-0.016583	1473.5526	1601.8332	1740.6843
	O	-1.947164	0.021736	-0.076506	3364.8022	3834.7358	3947.5767
	H	-2.726330	-0.050812	0.479297			
	H	-1.605810	0.916166	0.029466			
cis-HONO-WD	N	1.736325	0.585748	0.018625	34.5621	100.4578	125.6849
	O	1.603113	-0.728368	-0.033893	167.5002	181.7461	210.4327
	O	0.711635	1.190239	0.035121	220.4845	268.7695	317.4002
	H	0.629782	-0.98796	-0.039639	401.7705	463.725	704.8529
	O	-2.155682	0.819729	-0.074453	777.0812	1009.4344	1125.3684
	H	-1.282722	1.226202	-0.009713	1494.0458	1606.2442	1639.6406
	H	-2.779708	1.409241	0.351756	1709.0784	3041.7907	3627.0145
	O	-0.908281	-1.605882	-0.053815	3811.7069	3927.3651	3951.1711
	H	-1.164712	-2.267241	0.591744			
H	-1.563187	-0.886222	-0.008207				
trans-HONO-WM	N	-1.256053	-0.133790	-0.313482	21.0411	42.2116	127.7496
	O	-0.648233	1.016990	0.199513	138.2001	169.0799	353.9045
	O	-0.789070	-1.085823	0.155247	571.9561	697.8119	880.9137
	H	-1.080641	1.743291	-0.268761	1331.3135	1627.9115	1843.7424
	O	2.222275	0.021601	-0.102957	3826.1442	3855.9378	3952.8957
	H	2.160866	-0.881929	0.213642			
	H	1.432375	0.453020	0.23507			
trans-HONO-WD	N	-1.724475	0.41749	0.151690	16.9262	75.3704	123.797
	O	-0.540401	-0.045714	-0.364193	135.2253	165.6112	206.4476
	O	-2.560771	-0.395289	0.105131	224.6619	254.4071	274.9122
	H	0.109382	0.690513	-0.252989	388.2484	466.1589	679.7725
	O	1.986142	-1.320842	0.158616	765.5282	921.7129	959.2054
	H	1.040303	-1.412495	-0.013370	1466.0205	1616.4012	1627.0178
	H	2.423583	-1.991983	-0.369103	1817.1194	3364.0387	3681.1198
	O	1.674682	1.418585	-0.050458	3801.8519	3930.7305	3939.8068
	H	1.900817	1.972963	0.698921			
H	2.120016	0.564653	0.081933				
Cl-WM	C	-0.797098	1.017621	-0.169000	110.0571	171.179	222.4623
	H	-1.289634	1.87323	0.275769	227.2284	435.6982	535.1828
	O	-1.087843	-0.076611	0.324367	683.1774	714.8774	895.9509
	O	-0.473713	-1.185961	-0.185845	1080.1801	1270.1252	1455.4179
	H	-0.087827	1.067076	-0.986932	1640.7768	1662.8201	3140.7315
	O	1.853688	0.211666	0.016441	3286.5306	3550.577	3936.821
	H	2.591074	-0.10064	0.542576			
H	1.231917	-0.538143	-0.057126				



compound	Cartesian coordinate(Å)			frequency(cm <sup>-1</sup> )			
CI-WD	C	-0.99447	1.135818	0.159284	41.789	97.4814	160.6923
	H	-0.794513	1.072527	1.22165	216.6512	230.8245	270.7968
	H	-1.009016	2.057106	-0.406697	286.7935	293.3305	449.2186
	O	-1.281167	0.109426	-0.459071	478.0156	525.5965	720.3481
	O	-1.252019	-1.073791	0.279876	834.7527	863.5392	971.9557
	O	1.361202	-1.392561	0.023324	1110.8924	1255.4107	1448.0697
	H	0.3756	-1.432483	0.136507	1632.9744	1661.7515	1686.0854
	H	1.574245	-1.979577	-0.703903	3156.6415	3185.1121	3299.6805
	O	1.437603	1.295324	-0.050003	3411.8486	3920.9437	3928.6186
	H	1.567026	0.320167	-0.07523			
H	2.128521	1.640172	0.518954				
RC <sub>unc</sub>	O	1.432993	-1.144409	0.153765	29.3392	89.2185	105.997
	O	1.983689	-0.052822	-0.463434	156.3452	166.5127	258.9553
	C	1.875536	1.03995	0.100942	539.422	694.0269	764.4053
	H	2.309294	1.881652	-0.424708	888.5999	964.2469	1041.582
	H	1.369229	1.102514	1.05852	1090.8326	1266.752	1439.2134
	N	-1.880012	-0.369376	-0.242632	1459.304	1664.7057	1806.2324
	O	-0.830421	0.084835	0.506977	3091.3709	3135.9082	3281.578
	H	-0.095611	-0.583808	0.382315			
O	-2.795766	0.355592	-0.187728				
RC <sub>cis-HONO-WM</sub> <sup>HAT</sup>	C	-0.496156	-0.580363	-1.055982	51.6324	72.8583	92.9749
	H	-0.548275	-1.004732	-2.053277	107.7352	114.0658	188.3751
	O	-0.951279	-1.335447	-0.164885	192.9571	207.6148	241.3837
	O	-0.652712	-0.829547	1.114353	285.2275	351.2689	533.7014
	N	2.121972	0.454435	-0.110746	569.0157	705.8774	758.5568
	O	1.561918	-0.70351	0.033777	880.6592	1021.0363	1058.5222
	O	1.396576	1.393962	0.119025	1140.266	1288.9835	1471.2737
	H	0.387054	-0.678658	0.911968	1509.9675	1623.6103	1664.2566
	H	-0.211911	0.441285	-0.839497	1737.3376	2910.8582	3093.8136
	O	-2.265374	1.265855	-0.061307	3254.9123	3753.4707	3923.6978
	H	-1.917506	0.988181	0.793593			
	H	-2.299257	2.224559	-0.029376			
RC <sub>cis-HONO-WD</sub> <sup>HAT</sup>	C	1.190899	-0.893387	1.183517	26.3112	41.3534	71.4733
	H	1.670417	-1.330379	2.053322	83.4998	106.9915	120.7699
	O	1.281338	-1.57845	0.158903	174.0614	193.5053	214.2513
	O	0.680724	-1.065946	-0.985395	219.1437	226.9471	240.3952
	N	-2.448542	-0.019613	0.082268	286.6656	305.7332	377.7149
	O	-1.666834	-1.102298	0.161408	425.7893	547.722	658.6053
	O	-2.079513	0.786361	-0.701802	742.9256	746.1856	756.8695
	H	-0.876796	-1.000677	-0.463765	885.1324	1043.2498	1070.7831
	H	0.668987	0.069523	1.175168	1191.7722	1277.5024	1469.6176
	O	0.132581	1.964017	1.001246	1480.4018	1614.0888	1644.2493

	H	-0.699284	2.162489	0.562884	1672.4784	1721.4743	2940.8839
	H	0.814401	2.043082	0.315956	3026.6831	3231.4937	3539.8102
	O	2.148166	1.20147	-0.736724	3718.8733	3903.969	3933.7787
	H	1.64246	0.454852	-1.112992			
	H	2.802515	1.457484	-1.388631			
$RC_{trans-HONO-WM}^{HAT}$	C	0.362467	0.682448	0.901057	42.1718	64.1998	87.502
	H	0.608937	1.222162	1.812028	128.7622	133.6321	154.2084
	O	-0.28366	1.626058	0.10215	183.6659	193.2102	255.7933
	O	-0.760474	0.951695	-1.055413	307.941	379.8174	530.3174
	N	1.660508	-0.954337	-0.331051	590.8488	695.5904	769.0961
	O	1.592814	0.290598	0.315982	880.8467	998.875	1045.5866
	H	-0.199422	1.324194	-1.746971	1130.1232	1261.4086	1461.8893
	H	-0.278823	-0.17499	1.089517	1555.3241	1619.375	1688.3073
	O	-2.441331	-0.97242	0.420295	1798.4696	3039.2332	3149.6617
	H	-2.134381	-1.829903	0.11741	3294.988	3692.3941	3940.3336
	H	-2.186664	-0.35979	-0.277841			
	O	0.691651	-1.59543	-0.293405			
$RC_{trans-HONO-WD}^{HAT}$	C	2.243979	2.497913	0.63895	33.3424	59.3733	66.2554
	H	1.450344	3.040729	1.141717	84.0959	110.7622	139.3783
	H	3.304371	2.653102	0.791431	150.3927	183.4357	206.2628
	O	1.945819	1.621944	-0.177256	229.728	252.0782	285.7093
	O	0.629067	1.389727	-0.40372	321.0801	363.1218	407.2697
	N	-2.633162	0.282129	0.578774	489.0763	529.1405	747.4006
	O	-2.042744	0.475859	-0.658399	771.5146	790.9336	886.056
	O	-3.545941	-0.469793	0.516914	921.9016	1028.2688	1054.1251
	H	-1.307648	1.081488	-0.476277	1130.7963	1253.3169	1451.2502
	O	0.548696	-1.416704	-0.738471	1564.1764	1622.6956	1647.3297
	H	0.591932	-0.449616	-0.675635	1673.6545	1793.2738	2979.2209
	H	-0.162121	-1.600146	-1.355917	3175.0568	3316.6346	3358.8869
	O	2.190613	-3.438472	0.477544	3467.1017	3912.4755	3929.4294
	H	1.633121	-2.756267	0.075343			
	H	1.654181	-4.232157	0.481337			
$RC_{cis-HONO-WM}^{OAT}$	O	0.431715	1.431715	0.657574	33.2158	64.7771	76.2672
	O	1.165336	-0.985989	-0.480483	136.4359	153.7481	175.9441
	C	2.229679	-0.407902	-0.253004	202.5597	241.6534	294.3435
	H	2.809728	-0.124568	-1.121934	299.9111	378.3229	552.2047
	H	2.551144	-0.267423	0.770841	611.7938	731.6896	781.5566
	N	-2.296195	0.342606	-0.206818	892.3795	1128.5001	1177.3488
	O	-1.974175	-0.909214	-0.018647	1242.6279	1262.1418	1450.648
	O	-1.40379	1.128248	-0.057819	1502.7628	1633.4903	1649.7576
	O	1.351068	1.758128	0.263187	1693.1381	2399.1767	3156.045
	H	0.427399	1.466004	0.335217	3299.1806	3704.63587	3920.4664
	H	-0.968529	-1.022903	0.249986			
	H	1.314318	2.609424	-0.178856			

compound	Cartesian coordinate(Å)			frequency(cm <sup>-1</sup> )			
RC <sup>OAT</sup> <sub>cis-HONO-WD</sub>	O	0.066104	-0.888321	0.946375	32.2996	43.4628	59.4677
	O	0.631311	-1.11846	-0.322491	80.6005	113.97	134.3993
	C	1.841891	-1.369491	-0.303291	138.7453	222.8683	241.5706
	H	2.29825	-1.573172	-1.261593	251.914	267.8315	287.8588
	H	2.336496	-1.505773	0.649308	336.2342	364.0409	427.8116
	N	-2.773672	0.246616	-0.43938	535.4577	555.358	751.8357
	O	-2.445508	-0.838529	0.244882	765.5615	792.4757	885.8985
	O	-1.89017	1.031212	-0.578035	989.0751	1116.4449	1129.9667
	O	0.700608	1.796104	0.640358	1159.6876	1254.8401	1449.1414
	H	0.324838	0.941666	0.928019	1489.3516	1633.1545	1654.8092
	H	0.014895	2.171275	0.079831	1679.5465	1705.1037	2776.1897
	O	2.831427	0.656514	-0.429383	3166.4398	3222.4261	3308.6157
	H	3.617938	0.935533	0.045643	3580.5329	3892.9875	3906.1749
	H	2.085592	1.213501	-0.0857			
H	-1.463817	-0.800551	0.526246				
RC <sup>OAT</sup> <sub>trans-HONO-WM</sub>	O	-2.431613	-0.083413	0.080006	19.5347	27.9408	83.5884
	O	-1.548534	-0.989039	-0.493349	105.4524	144.8179	156.9422
	C	-0.753515	-1.531925	0.275666	219.3817	262.5549	290.5811
	H	-0.049034	-2.223683	-0.170344	301.4177	521.8913	558.6657
	H	-0.807015	-1.313322	1.335726	721.1643	773.7072	824.7754
	N	2.151023	0.382839	-0.248067	872.3713	972.9461	1113.0119
	O	1.018198	0.282675	0.502216	1120.4312	1250.6285	1446.3102
	O	2.819061	-0.574563	-0.150046	1469.24	1668.5734	1683.6944
	H	0.442362	1.081191	0.277244	1794.1749	2934.5576	3143.8775
	O	-0.796806	1.974774	-0.140699	3182.4481	3287.4663	3928.8452
	H	-1.544732	1.320333	-0.081264			
	H	-1.060103	2.763682	0.336087			
RC <sup>OAT</sup> <sub>trans-HONO-WD</sub>	O	-1.831801	-1.363888	-0.615627	25.6065	60.0305	68.0513
	O	-2.414468	-0.096203	-0.729797	74.6629	100.4945	113.1461
	C	-1.646435	0.819952	-1.037555	142.1348	170.7908	188.5482
	H	-2.094861	1.79824	-1.14419	245.3723	273.9449	302.892
	H	-0.604945	0.597343	-1.247679	353.4464	374.4019	447.1659
	N	2.658323	-0.485	-0.126231	523.5883	583.0445	686.8457
	O	1.478164	0.181578	0.087801	752.2933	766.4865	877.1865
	O	3.388281	0.136592	-0.792466	931.5643	957.3322	1084.9106
	H	0.923282	-0.420984	0.650165	1135.1621	1259.8456	1453.884
	O	-0.422615	-1.014717	1.463955	1464.2929	1645.5445	1674.758
	H	-1.030051	-1.263449	0.681946	1680.4659	1815.176	2710.8746
	H	-0.45052	-1.725308	2.106946	3142.5115	3255.3668	3290.9893
	O	-0.79918	1.73819	1.039259	3712.4853	3874.6265	3925.4635
	H	0.134243	1.942714	0.917658			
	H	-0.793855	0.894325	1.519101			

compound	Cartesian coordinate(Å)			frequency(cm <sup>-1</sup> )			
TS <sup>OAT</sup> <sub>cis-HONO-WM</sub>	O	0.205758	-0.604827	-0.150844	-662.7351	24.9058	56.1177
	O	1.81586	-0.979435	-0.571166	67.9441	113.06	160.8101
	C	2.56958	-0.615361	0.300471	178.9455	185.8344	235.4462
	H	3.646149	-0.745851	0.154676	341.3648	387.7433	449.5104
	H	2.185806	-0.165078	1.217506	535.6229	548.4694	663.0577
	N	-1.584982	-0.247187	0.143264	707.9277	742.2869	984.3175
	O	-2.001065	0.912063	-0.428418	1202.1284	1256.9179	1381.8725
	O	-2.43494	-0.989006	0.440576	1494.3605	1649.47	1790.7055
	O	1.303795	1.877085	0.270134	1802.4148	3047.76	3165.3322
	H	0.727601	1.120222	0.042264	3515.1592	3670.689	3936.8971
	H	-2.974889	0.864562	-0.465399			
	H	0.977457	2.621578	-0.236989			
	TS <sup>OAT</sup> <sub>cis-HONO-WD</sub>	O	0.333492	-0.575585	0.304761	-657.3503	23.7703
O		-1.164766	-1.140935	0.926675	54.8312	88.9187	102.2188
C		-1.886063	-1.463883	0.008576	151.3309	188.9093	204.6116
H		-2.888166	-1.837641	0.222197	226.6268	239.9186	265.4359
H		-1.522678	-1.416257	-1.01828	285.6325	389.136	429.1706
N		2.011676	-0.108544	-0.26001	450.9471	460.7794	519.4422
O		2.617828	0.794453	0.544226	601.5302	671.0921	715.4677
O		2.722643	-0.716509	-0.959244	805.7719	959.1317	1003.4298
O		-0.7896	1.837989	0.124412	1192.0928	1248.2988	1389.5676
H		-0.28745	0.990279	0.22752	1485.2704	1636.3633	1658.539
H		-0.698432	2.301844	0.958555	1784.6855	1784.9749	3074.42
O		-3.112239	0.622942	-0.595143	3185.604	3237.1072	3462.7603
H		-3.448288	1.006156	-1.407223	3670.4615	3925.5817	3927.2872
H		-2.351403	1.182525	-0.328365			
H	3.572178	0.73737	0.34872				
TS <sup>OAT</sup> <sub>trans-HONO-WM</sub>	O	0.622396	-0.081215	-0.068341	-588.5556	44.1947	62.6929
	O	2.243784	0.352263	-0.064982	89.2339	152.5587	202.2913
	C	2.916696	-0.639006	0.087962	235.1219	270.6154	354.0464
	H	4.005145	-0.540956	0.113432	361.6148	377.6774	477.0292
	H	2.428242	-1.610637	0.197232	533.2732	565.7825	775.3988
	N	-1.23674	-0.71781	-0.029256	965.5977	1043.7314	1076.5643
	O	-2.259241	0.130059	0.090536	1206.6536	1246.9819	1475.7783
	O	-1.53863	-1.847093	-0.054101	1571.0728	1644.2169	1804.7658
	H	-1.813317	1.033366	0.094046	1823.0411	2943.0689	3047.2703
	O	-0.676162	2.173738	0.091481	3164.059	3172.6131	3922.3644
	H	-0.00254	1.441069	0.012722			
	H	-0.597708	2.713842	-0.697165			

compound	Cartesian coordinate(Å)			frequency(cm <sup>-1</sup> )			
TS <sup>OAT</sup> <sub>trans-HONO-WD</sub>	O	-0.194805	0.824675	0.390252	-597.2945	42.0853	57.657
	O	1.415647	1.297491	0.724365	107.3479	128.2362	142.3938
	C	2.03181	1.371645	-0.315965	158.6948	175.1211	208.2871
	H	3.095212	1.615636	-0.286866	234.2947	273.0022	297.4539
	H	1.523194	1.225578	-1.268438	353.0973	389.7393	438.4844
	N	-1.946568	0.239182	-0.111313	458.1164	514.74	558.8572
	O	-2.17225	-1.079564	-0.260581	592.7272	718.0694	763.1242
	O	-2.832687	0.919101	-0.437667	931.2064	1027.5345	1196.6166
	H	-1.335545	-1.503095	0.065156	1235.9262	1248.6544	1485.5582
	O	0.260552	-1.620144	0.703242	1535.6802	1608.4779	1645.528
	H	0.147052	-0.595188	0.701966	1786.8093	1841.0669	2547.0104
	H	0.336452	-1.905613	1.616519	3074.2284	3188.5196	3271.1709
	O	2.63921	-1.047502	-0.686698	3633.3732	3909.2367	3929.7413
	H	2.877868	-1.664292	-1.381041			
	H	1.86554	-1.429631	-0.23562			
TS <sup>HAT</sup> <sub>cis-HONO-WM</sub>	C	-0.496156	-0.580363	-1.055982	-345.3161	23.5011	90.3477
	H	-0.548275	-1.004732	-2.053277	132.1229	157.099	173.6952
	O	-0.951279	-1.335447	-0.164885	176.5501	196.6968	251.8712
	O	-0.652712	-0.829547	1.114353	345.5896	399.4891	429.1786
	N	2.121972	0.454435	-0.110746	575.094	759.2135	828.2715
	O	1.561918	-0.70351	0.033777	949.8135	1095.2665	1135.7951
	O	1.396576	1.393962	0.119025	1168.1828	1266.5881	1439.6894
	H	0.387054	-0.678658	0.911968	1478.6408	1591.4154	1617.4709
	H	-0.211911	0.441285	-0.839497	1628.5032	2249.0876	3134.9387
	O	-2.265374	1.265855	-0.061307	3282.6287	3828.6331	3941.1745
	H	-1.917506	0.988181	0.793593			
	H	-2.299257	2.224559	-0.029376			
TS <sup>HAT</sup> <sub>cis-HONO-WD</sub>	C	0.323947	-0.987738	1.184245	-358.1694	28.1199	38.0907
	H	0.224566	-1.47139	2.151271	59.4073	115.8296	143.3439
	O	0.652187	-1.780847	0.266449	153.7154	171.7589	197.3067
	O	0.492721	-1.162129	-0.993632	211.3758	225.9054	281.4576
	N	-2.255075	0.377596	-0.031754	352.4943	370.3739	395.6576
	O	-1.64855	-0.764297	0.114955	476.4918	506.7169	572.4257
	O	-1.709848	1.128767	-0.798037	649.0689	793.3061	824.4117
	H	-0.533844	-0.861857	-0.798071	944.4885	1081.6313	1161.1862
	H	0.31563	0.098514	1.045154	1191.5748	1265.4286	1358.9003
	O	0.515794	1.981455	0.882776	1461.5486	1603.3974	1608.2306
	H	-0.188411	2.204262	0.263431	1626.2859	1639.2284	2141.0713
	H	1.320386	1.897697	0.352054	2999.5919	3229.9341	3754.7138
	O	2.601178	0.666198	-0.466713	3785.187	3865.3288	3937.8884
	H	2.039627	0.101854	-1.014095			
	H	3.436044	0.761004	-0.929318			

compound	Cartesian coordinate(Å)			frequency(cm <sup>-1</sup> )			
TS <sup>HAT</sup> <sub>trans-HONO-WM</sub>	C	1.131851	1.097046	-0.127723	-207.8178	54.6514	72.2237
	H	0.913161	2.006147	0.419037	124.0961	149.2527	161.7606
	O	2.045577	0.389644	0.338572	178.9882	213.1795	293.9617
	O	2.148541	-0.859837	-0.325391	380.0103	428.6608	556.8002
	N	-1.227981	-1.469285	-0.038051	657.2314	710.3583	876.4599
	O	-0.176258	-0.804937	0.312994	919.592	1037.959	1139.2114
	H	1.14691	-1.165879	-0.110016	1162.2381	1229.7043	1427.799
	H	0.654944	0.853482	-1.065925	1558.9027	1595.0772	1640.584
	O	-1.401387	1.908748	-0.057427	1658.9589	2194.0293	3176.3201
	H	-1.749868	1.006407	0.069172	3320.9038	3593.8469	3930.1861
	H	-2.166915	2.481339	-0.130982			
	O	-2.240657	-0.818464	-0.037322			
	TS <sup>HAT</sup> <sub>trans-HONO-WD</sub>	C	0.092302	-0.914696	1.092963	-663.9137	28.0429
H		-0.366987	-1.364297	1.966975	61.6382	91.9094	110.5355
O		0.835092	-1.705964	0.429485	125.0234	167.5654	176.2259
O		1.051104	-1.124923	-0.860897	197.6615	227.151	233.4882
N		-1.936671	0.305857	-0.662842	293.9531	381.7817	400.5019
O		-1.256995	-0.862073	-0.330257	418.4713	532.3159	671.1982
H		-0.309584	-0.911022	-0.9141	733.0329	773.7968	862.6244
H		0.190473	0.162578	0.986875	890.1205	930.2354	1041.2444
O		0.230878	2.090864	0.362288	1247.4053	1259.9308	1342.566
H		-0.172618	2.673441	-0.283442	1428.9206	1584.8769	1616.6597
H		1.163855	1.992864	0.108519	1633.2298	1812.5573	2013.9776
O		2.653354	0.941914	-0.134985	3114.8989	3253.9635	3504.9325
H		2.23741	0.150141	-0.531435	3675.9788	3933.8795	3943.4218
O	3.580837	0.934129	-0.373802				
O	-2.678495	0.62385	0.174681				
PC <sup>OAT</sup> <sub>cis-HONO-WM</sub>	O	-1.88332	-0.681543	-0.068223	62.9315	70.2331	82.7143
	O	1.469252	-1.143642	0.409333	99.8344	125.2911	143.0814
	C	0.819444	-1.979443	-0.163024	193.4142	215.1022	272.3164
	H	0.614512	-2.95321	0.304246	285.9425	420.1416	604.3872
	H	0.402899	-1.799083	-1.164126	681.4096	722.1466	841.1204
	N	-1.153944	0.260939	0.059195	1024.0056	1061.4406	1229.4761
	O	-0.539808	0.666903	-1.072734	1280.6418	1416.4979	1510.2125
	O	-0.906436	0.867052	1.07005	1542.6631	1637.0292	1772.5446
	O	1.670518	1.633388	-0.161673	1842.7576	2916.3993	2991.6762
	H	1.903651	0.733202	0.11975	3082.0797	3713.9838	3897.8343
	H	0.256072	1.210767	-0.760381			
H	1.502166	2.121147	0.650272				

compound	Cartesian coordinate(Å)			frequency( $\text{cm}^{-1}$ )			
$\text{PC}_{cis-HONO-WD}^{OAT}$	O	-2.708923	0.727727	0.738475	27.5965	40.3449	70.2437
	O	2.959764	-0.089428	0.399089	92.3741	103.5974	111.7754
	C	2.383626	0.904051	0.766538	131.9312	148.5391	156.8832
	H	2.87831	1.884019	0.742246	206.5134	226.7443	249.1071
	H	1.353491	0.870693	1.143451	273.3059	307.0317	328.6904
	N	-1.924428	0.009327	0.201315	486.8507	507.939	663.302
	O	-0.981804	-0.523356	1.011973	722.2656	746.7185	837.6621
	O	-1.875056	-0.297145	-0.966797	991.6163	1025.8103	1223.8378
	O	0.918459	-1.623975	-0.410229	1283.0045	1411.2321	1461.7727
	H	1.781522	-1.290447	-0.084528	1545.8585	1617.6056	1629.3595
	H	1.014613	-2.550173	-0.640325	1780.4911	1831.4432	3004.8485
	O	0.689536	1.159972	-1.324156	3096.9121	3112.2541	3473.3854
	H	-0.088385	1.572054	-1.708337	3811.0318	3923.5146	3927.0793
	H	0.561265	0.213764	-1.464664			
	H	-0.347379	-1.019856	0.416873			
$\text{PC}_{trans-HONO-WM}^{OAT}$	O	0.436944	-0.812614	-0.089229	37.2272	52.0608	69.6122
	O	-2.643307	-0.025536	0.191553	78.2895	122.44	168.6824
	C	-2.582879	-1.195757	-0.08194	180.3468	203.4158	264.5299
	H	-3.446606	-1.85386	0.09389	302.5245	478.3956	672.1468
	H	-1.674935	-1.640674	-0.507072	721.3259	727.7706	840.9897
	N	1.567292	-0.378602	0.005765	981.1311	1047.1122	1238.5385
	O	1.705146	0.954977	0.02336	1286.9689	1410.1915	1537.0731
	O	2.576187	-1.007827	0.086315	1542.5584	1642.6907	1790.5559
	H	0.765743	1.335337	-0.042261	1843.1179	2876.9606	2994.5609
	O	-0.677244	1.908329	-0.144352	3098.0474	3575.492	3924.8607
	H	-1.33404	1.195278	-0.02577			
	H	-0.965743	2.650034	0.39133			
$\text{PC}_{trans-HONO-WD}^{OAT}$	O	0.702805	-0.749804	-0.383919	-32.3285	39.3926	47.6063
	O	-2.192249	-0.530836	1.13177	71.8919	78.7142	92.3548
	C	-2.355562	-1.339325	0.251537	116.8618	151.2743	163.0409
	H	-2.906934	-2.26871	0.453173	184.2474	198.6761	226.2046
	H	-1.972075	-1.163684	-0.760209	286.9786	350.467	360.7375
	N	1.786636	-0.355507	0.003264	459.9478	551.5989	687.4561
	O	1.812113	0.842863	0.609864	725.386	828.6054	841.7552
	O	2.833623	-0.910893	-0.094032	981.0617	1041.3743	1243.1138
	H	0.854524	1.162916	0.638329	1291.1836	1403.7551	1530.9769
	O	-0.66066	1.647284	0.693238	1539.1567	1643.7644	1650.1998
	H	-1.21893	0.853393	0.866331	1791.0506	1828.5022	2960.3488
	H	-0.919088	2.319646	1.328436	2998.2618	3114.6131	3377.0463
	O	-1.311609	0.70568	-2.042316	3830.8053	3906.0975	3911.8271
	H	-0.481126	0.220752	-2.025531			
	H	-1.201638	1.365833	-1.349429			

compound	Cartesian coordinate(Å)			frequency(cm <sup>-1</sup> )			
PC <sup>HAT</sup> <sub>cis-HONO-WM</sub>	C	0.35807	-0.681476	-0.901439	45.7938	77.2556	107.5965
	H	0.600665	-1.220481	-1.813915	123.0879	130.6272	154.0945
	O	-0.289055	-1.62426	-0.102338	225.2284	240.3128	248.7398
	O	-0.76121	-0.949985	1.057252	351.4819	431.4096	458.2311
	N	1.664394	0.949236	0.329777	594.5138	698.3387	891.762
	O	1.591106	-0.294509	-0.318647	959.8193	1012.6139	1117.6373
	O	0.697477	1.593491	0.295438	1183.4288	1325.9992	1407.1963
	H	-0.19916	-1.324647	1.74682	1430.5781	1496.0269	1630.4613
	H	-0.281074	0.178289	-1.086931	1803.1363	3123.1607	3190.0186
	O	-2.438527	0.977354	-0.420312	3825.8749	3835.676	3939.3747
	H	-2.189135	0.361722	0.27707			
	H	-2.128817	1.832593	-0.113995			
	PC <sup>HAT</sup> <sub>cis-HONO-WD</sub>	C	-0.264504	0.41919	0.582305	22.5055	25.2341
H		0.281395	0.978138	1.335522	110.7585	120.068	159.482
O		-0.185426	-0.940322	0.894721	160.2219	193.6818	213.603
O		0.077644	-1.709063	-0.267628	227.2673	264.5139	280.2285
N		-2.514962	0.573457	-0.225759	339.91	373.9821	410.6575
O		-1.604567	0.919486	0.714153	468.1901	553.5536	561.8399
O		-2.14267	-0.214236	-1.020339	690.4434	771.998	930.2364
H		-0.749552	-1.640513	-0.769083	973.5932	1003.6749	1126.947
H		0.125677	0.62022	-0.41231	1154.4919	1332.194	1420.9383
O		2.193294	1.877243	-0.347117	1443.5859	1461.7848	1632.8654
H		2.855954	2.425911	-0.769368	1642.285	1728.9386	3130.9809
H		2.56625	0.981526	-0.31112	3204.7739	3675.9813	3767.8954
O		2.797648	-0.857068	-0.142202	3780.4391	3927.4702	3938.2884
H	1.96922	-1.30663	-0.357722				
H	3.055434	-1.196314	0.71786				
PC <sup>HAT</sup> <sub>trans-HONO-WM</sub>	C	-0.373943	0.338838	-0.210442	28.2609	68.7682	89.8523
	H	0.30915	0.70937	-0.971878	134.7105	153.1824	165.375
	O	-1.621754	0.829008	-0.512537	195.5537	266.7395	291.818
	O	-2.466912	0.576545	0.600701	317.8242	348.2428	422.0009
	N	0.627187	-1.817113	3.2×10 <sup>-05</sup>	566.1786	805.1337	964.8631
	O	-0.476777	-1.105097	-0.287113	992.5468	1034.3555	1127.3444
	H	-2.884748	-0.25783	0.348748	1188.8711	1306.5444	1415.971
	H	-0.046687	0.621894	0.788275	1433.0755	1476.8963	1608.8263
	O	2.330251	1.703325	0.042147	1717.5682	3106.874	3179.1476
	H	2.51423	0.779966	0.23764	3807.3075	3852.6993	3958.9939
	H	3.16069	2.169175	0.156576			
	O	1.585281	-1.170757	0.244685			



compound	Cartesian coordinate(Å)			frequency(cm <sup>-1</sup> )			
<i>PC<sup>HAT</sup><sub>trans-HONO-WD</sub></i>	C	-2.051206	0.582435	0.002964	33.3505	64.9223	77.5755
	O	-2.121157	-0.78604	-0.111801	97.5754	120.1146	143.3446
	O	-0.834394	1.081116	-0.562307	149.3599	204.5044	216.4593
	O	-1.260398	-1.341465	0.872622	233.2818	277.9893	296.8189
	N	0.099099	1.330148	0.411283	334.0892	359.605	437.9544
	O	1.134989	1.598144	-0.064302	467.1753	559.324	681.7459
	H	-2.856182	0.982239	-0.608041	736.2126	784.2782	892.8559
	H	-2.105895	0.903474	1.042632	971.9914	1075.089	1160.1214
	H	-0.456078	-1.533062	0.336147	1201.377	1334.8895	1425.2974
	H	0.63133	-0.924623	-1.501544	1481.5917	1575.3734	1607.2649
	H	1.722345	-1.221671	-0.449897	1641.2701	1786.2298	3101.9275
	H	2.958335	0.526728	0.486977	3180.2692	3402.5702	3672.1487
	H	4.098593	-0.456774	0.150527	3843.9236	3901.191	3953.936
	O	0.868211	-1.53165	-0.794963			
	O	3.165386	-0.405349	0.366555			
HNO <sub>3</sub>	O	-1.055546	-0.718561	-0.000172	507.2984	621.9768	706.3832
	N	-0.140911	0.035973	0.000136	825.2843	983.1121	1359.1869
	O	1.09695	-0.571722	0.000258	1415.6371	1808.505	3779.9411
	O	-0.13275	1.237065	5.2×10 <sup>-05</sup>			
	H	1.717148	0.173924	-0.002052			
CH <sub>2</sub> O	O	0.670376	-8.3×10 <sup>-05</sup>	7×10 <sup>-06</sup>	1213.3136	1274.14	1539.5236
	C	-0.525586	3×10 <sup>-06</sup>	-2.9×10 <sup>-05</sup>	1869.3614	2944.8969	3015.8701
	H	-1.104128	0.939254	5.9×10 <sup>-05</sup>			
	H	-1.105367	-0.938613	5.9×10 <sup>-05</sup>			
CH <sub>3</sub> NO <sub>4</sub> (HPMN)	C	-0.56368	0.890853	0.204982	79.735	156.3855	182.7558
	H	-1.067181	1.191554	1.120593	265.5722	331.2679	460.7702
	H	-0.209139	1.739056	-0.379333	576.7098	705.3853	837.4167
	O	-1.428301	0.203462	-0.635105	963.2505	1093.2376	1133.4987
	O	-2.12589	-0.748955	0.153027	1198.5341	1335.1726	1416.547
	O	0.52709	0.082189	0.602201	1427.9949	1478.4295	1846.4026
	N	1.566402	0.181558	-0.340685	3104.6829	3174.7255	3807.7072
	O	2.433983	-0.538772	-0.078309			
H	-1.561475	-1.530021	0.079135				

Table S2: Termolecular rate constant  $k_t$  in ( $\text{cm}^6 \text{ molecule}^{-2} \text{ sec}^{-1}$ ) for  $\text{H}_2\text{O}$  catalyzed channels for OAT path for  $\text{CH}_2\text{OO} + \text{cis-HONO}$  within temperature range 213-320K.

Temp (K)	PATH A				PATH B				PATH C			
	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt
213	1.66E-18	5.76E-18	1.15E-12	1.10E-47	7.88E-20	1.21E-16	1.15E-12	1.10E-47	4.38E-19	2.19E-17	1.15E-12	1.10E-47
216	1.28E-18	4.31E-18	2.53E-12	1.39E-47	6.48E-20	8.48E-17	2.53E-12	1.39E-47	3.47E-19	1.58E-17	2.53E-12	1.39E-47
219	9.88E-19	3.25E-18	5.46E-12	1.75E-47	5.36E-20	5.99E-17	5.46E-12	1.75E-47	2.77E-19	1.16E-17	5.46E-12	1.75E-47
224	6.55E-19	2.07E-18	1.89E-11	2.56E-47	3.95E-20	3.42E-17	1.89E-11	2.56E-47	1.93E-19	7.02E-18	1.89E-11	2.56E-47
235	2.83E-19	8.17E-19	2.41E-10	5.58E-47	2.12E-20	1.09E-17	2.41E-10	5.58E-47	9.20E-20	2.52E-18	2.41E-10	5.58E-47
250	1.03E-19	2.65E-19	5.51E-09	1.49E-46	9.99E-21	2.72E-18	5.51E-09	1.49E-46	3.74E-20	7.25E-19	5.51E-09	1.49E-46
259	5.92E-20	1.44E-19	3.04E-08	2.58E-46	6.65E-21	1.28E-18	3.04E-08	2.58E-46	2.30E-20	3.69E-19	3.04E-08	2.58E-46
265	4.20E-20	9.77E-20	8.93E-08	3.66E-46	5.15E-21	7.96E-19	8.93E-08	3.66E-46	1.69E-20	2.42E-19	8.93E-08	3.66E-46
278	2.10E-20	4.52E-20	7.90E-07	7.50E-46	3.09E-21	3.07E-19	7.90E-07	7.50E-46	9.17E-21	1.04E-19	7.90E-07	7.50E-46
280	1.90E-20	4.04E-20	1.09E-06	8.37E-46	2.87E-21	2.67E-19	1.09E-06	8.37E-46	8.39E-21	9.15E-20	1.09E-06	8.37E-46
290	1.18E-20	2.36E-20	4.99E-06	1.39E-45	2.02E-21	1.38E-19	4.99E-06	1.39E-45	5.48E-21	5.08E-20	4.99E-06	1.39E-45
298	8.25E-21	1.58E-20	1.58E-05	2.06E-45	1.55E-21	8.41E-20	1.58E-05	2.06E-45	3.99E-21	3.27E-20	1.58E-05	2.06E-45
300	7.57E-21	1.43E-20	2.08E-05	2.26E-45	1.45E-21	7.46E-20	2.08E-05	2.26E-45	3.69E-21	2.94E-20	2.08E-05	2.26E-45
310	5.01E-21	9.00E-21	7.93E-05	3.58E-45	1.07E-21	4.20E-20	7.93E-05	3.58E-45	2.56E-21	1.76E-20	7.93E-05	3.58E-45
320	3.41E-21	5.83E-21	2.79E-04	5.55E-45	8.09E-22	2.46E-20	2.79E-04	5.56E-45	1.82E-21	1.10E-20	2.79E-04	5.55E-45

Table S3: Termolecular rate constant  $k_t$  in ( $\text{cm}^6 \text{ molecule}^{-2} \text{ sec}^{-1}$ ) for  $\text{H}_2\text{O}$  catalyzed channels for OAT path for  $\text{CH}_2\text{OO} + \text{trans-HONO}$  within temperature range 213-320K.

Temp (K)	PATH A				PATH B				PATH C			
	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt
213	6.19E-18	5.27E-17	3.38E-06	1.10E-39	3.10E-22	1.05E-12	3.38E-06	1.10E-39	4.38E-19	7.45E-16	3.38E-06	1.10E-39
216	4.58E-18	3.97E-17	5.77E-06	1.05E-39	2.93E-22	6.21E-13	5.77E-06	1.05E-39	3.47E-19	5.24E-16	5.77E-06	1.05E-39
219	3.42E-18	3.02E-17	9.71E-06	1.00E-39	2.77E-22	3.73E-13	9.71E-06	1.00E-39	2.77E-19	3.73E-16	9.71E-06	1.00E-39
224	2.14E-18	1.94E-17	2.25E-05	9.35E-40	2.53E-22	1.64E-13	2.25E-05	9.35E-40	1.93E-19	2.16E-16	2.25E-05	9.35E-40
235	8.21E-19	7.88E-18	1.26E-04	8.15E-40	2.11E-22	3.07E-14	1.26E-04	8.15E-40	9.20E-20	7.04E-17	1.26E-04	8.15E-40
250	2.57E-19	2.63E-18	1.05E-03	7.08E-40	1.71E-22	3.95E-15	1.05E-03	7.08E-40	3.74E-20	1.80E-17	1.05E-03	7.07E-40
259	1.37E-19	1.45E-18	3.32E-03	6.57E-40	1.53E-22	1.30E-15	3.32E-03	6.57E-40	2.30E-20	8.61E-18	3.32E-03	6.57E-40
265	9.21E-20	9.96E-19	6.88E-03	6.31E-40	1.43E-22	6.43E-16	6.88E-03	6.31E-40	1.69E-20	5.41E-18	6.88E-03	6.31E-40
278	4.17E-20	4.69E-19	3.00E-02	5.86E-40	1.25E-22	1.57E-16	3.00E-02	5.86E-40	9.17E-21	2.13E-18	3.00E-02	5.86E-40
280	3.71E-20	4.21E-19	3.72E-02	5.81E-40	1.23E-22	1.27E-16	3.72E-02	5.81E-40	8.39E-21	1.86E-18	3.72E-02	5.81E-40
290	2.14E-20	2.49E-19	1.04E-01	5.55E-40	1.12E-22	4.76E-17	1.04E-01	5.55E-40	5.48E-21	9.74E-19	1.04E-01	5.55E-40
298	1.42E-20	1.69E-19	2.26E-01	5.40E-40	1.05E-22	2.27E-17	2.26E-01	5.40E-40	3.99E-21	5.99E-19	2.26E-01	5.40E-40
300	1.29E-20	1.53E-19	2.73E-01	5.38E-40	1.04E-22	1.90E-17	2.73E-01	5.37E-40	3.69E-21	5.33E-19	2.73E-01	5.38E-40
310	7.98E-21	9.74E-20	6.72E-01	5.22E-40	9.64E-23	8.07E-18	6.72E-01	5.22E-40	2.56E-21	3.04E-19	6.72E-01	5.23E-40
320	5.12E-21	6.38E-20	1.57E+00	5.13E-40	9.04E-23	3.62E-18	1.57E+00	5.13E-40	1.82E-21	1.80E-19	1.57E+00	5.13E-40

Table S4: Termolecular rate constant  $k_t$  in ( $\text{cm}^6 \text{ molecule}^{-2} \text{ sec}^{-1}$ ) for  $(\text{H}_2\text{O})_2$  catalyzed channels for OAT path for  $\text{CH}_2\text{OO} + \text{cis-HONO}$  within temperature range 213-320K.

Temp (K)	PATH A				PATH B				PATH C			
	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt
213	1.66E-18	1.82E-14	1.02E-11	3.08E-43	1.06E-17	2.852E-15	1.02E-11	3.08E-43	6.50E-16	4.65E-17	1.02E-11	3.08E-43
216	1.28E-18	1.11E-14	2.21E-11	3.14E-43	7.60E-18	1.866E-15	2.21E-11	3.13E-43	4.28E-16	3.31E-17	2.21E-11	3.13E-43
219	9.88E-19	6.89E-15	4.68E-11	3.18E-43	5.51E-18	1.235E-15	4.68E-11	3.18E-43	2.86E-16	2.38E-17	4.68E-11	3.18E-43
224	6.55E-19	3.19E-15	1.58E-10	3.30E-43	3.28E-18	6.369E-16	1.58E-10	3.30E-43	1.49E-16	1.40E-17	1.58E-10	3.30E-43
235	2.83E-19	6.58E-16	1.91E-09	3.56E-43	1.14E-18	1.641E-16	1.91E-09	3.56E-43	3.92E-17	4.75E-18	1.91E-09	3.56E-43
250	1.03E-19	9.56E-17	4.08E-08	4.00E-43	3.12E-19	3.139E-17	4.08E-08	4.00E-43	7.70E-18	1.27E-18	4.08E-08	4.00E-43
259	5.92E-20	3.35E-17	2.17E-07	4.30E-43	1.55E-19	1.278E-17	2.17E-07	4.30E-43	3.18E-18	6.24E-19	2.17E-07	4.30E-43
265	4.20E-20	1.73E-17	6.24E-07	4.53E-43	9.99E-20	7.271E-18	6.24E-07	4.53E-43	1.82E-18	3.99E-19	6.24E-07	4.53E-43
278	2.10E-20	4.57E-18	5.28E-06	5.08E-43	4.12E-20	2.332E-18	5.28E-06	5.07E-43	5.93E-19	1.62E-19	5.28E-06	5.08E-43
280	1.90E-20	3.77E-18	7.21E-06	5.16E-43	3.62E-20	1.977E-18	7.21E-06	5.17E-43	5.03E-19	1.42E-19	7.21E-06	5.16E-43
290	1.18E-20	1.49E-18	3.21E-05	5.64E-43	1.96E-20	8.961E-19	3.21E-05	5.64E-43	2.30E-19	7.62E-20	3.21E-05	5.64E-43
298	8.25E-21	7.41E-19	9.90E-05	6.06E-43	1.24E-20	4.949E-19	9.90E-05	6.06E-43	1.28E-19	4.77E-20	9.90E-05	6.05E-43
300	7.57E-21	6.26E-19	1.30E-04	6.16E-43	1.11E-20	4.288E-19	1.30E-04	6.17E-43	1.11E-19	4.26E-20	1.30E-04	6.16E-43
310	5.01E-21	2.79E-19	4.82E-04	6.74E-43	6.49E-21	2.155E-19	4.82E-04	6.74E-43	5.63E-20	2.48E-20	4.82E-04	6.74E-43
320	3.41E-21	1.31E-19	1.65E-03	7.36E-43	3.94E-21	1.132E-19	1.65E-03	7.36E-43	2.98E-20	1.50E-20	1.65E-03	7.36E-43

Table S5: Termolecular rate constant  $k_t$  in ( $\text{cm}^6 \text{ molecule}^{-2} \text{ sec}^{-1}$ ) for  $(\text{H}_2\text{O})_2$  catalyzed channels for OAT path for  $\text{CH}_2\text{OO} + \text{trans-HONO}$  within temperature range 213-320K.

Temp (K)	PATH A				PATH B				PATH C			
	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt
213	6.19E-18	2.55E-16	2.96E-05	4.66E-38	1.48E-17	1.07E-16	2.96E-05	4.66E-38	6.50E-16	2.42E-18	2.96E-05	4.66E-38
216	4.58E-18	1.70E-16	4.91E-05	3.82E-38	1.08E-17	7.21E-17	4.91E-05	3.82E-38	4.28E-16	1.81E-18	4.91E-05	3.81E-38
219	3.42E-18	1.14E-16	8.04E-05	3.14E-38	7.94E-18	4.92E-17	8.04E-05	3.14E-38	2.86E-16	1.37E-18	8.04E-05	3.14E-38
224	2.14E-18	6.06E-17	1.78E-04	2.31E-38	4.86E-18	2.67E-17	1.78E-04	2.31E-38	1.49E-16	8.71E-19	1.78E-04	2.31E-38
235	8.21E-19	1.65E-17	9.11E-04	1.24E-38	1.78E-18	7.61E-18	9.11E-04	1.24E-38	3.92E-17	3.46E-19	9.11E-04	1.24E-38
250	2.57E-19	3.38E-18	6.75E-03	5.85E-39	5.26E-19	1.65E-18	6.75E-03	5.85E-39	7.70E-18	1.13E-19	6.75E-03	5.85E-39
259	1.37E-19	1.43E-18	2.02E-02	3.93E-39	2.71E-19	7.17E-19	2.02E-02	3.93E-39	3.18E-18	6.13E-20	2.02E-02	3.93E-39
265	9.21E-20	8.28E-19	4.02E-02	3.07E-39	1.79E-19	4.26E-19	4.02E-02	3.07E-39	1.82E-18	4.19E-20	4.02E-02	3.07E-39
278	4.17E-20	2.77E-19	1.62E-01	1.87E-39	7.77E-20	1.49E-19	1.62E-01	1.87E-39	5.93E-19	1.95E-20	1.62E-01	1.87E-39
280	3.71E-20	2.37E-19	1.99E-01	1.75E-39	6.88E-20	1.28E-19	1.99E-01	1.75E-39	5.03E-19	1.75E-20	1.99E-01	1.75E-39
290	2.14E-20	1.10E-19	5.28E-01	1.25E-39	3.85E-20	6.14E-20	5.28E-01	1.25E-39	2.30E-19	1.03E-20	5.28E-01	1.25E-39
298	1.42E-20	6.23E-20	1.10E+00	9.73E-40	2.49E-20	3.55E-20	1.10E+00	9.72E-40	1.28E-19	6.90E-21	1.10E+00	9.72E-40
300	1.29E-20	5.43E-20	1.31E+00	9.14E-40	2.24E-20	3.11E-20	1.31E+00	9.13E-40	1.11E-19	6.27E-21	1.31E+00	9.13E-40
310	7.98E-21	2.80E-20	3.09E+00	6.90E-40	1.36E-20	1.65E-20	3.09E+00	6.90E-40	5.63E-20	3.96E-21	3.09E+00	6.90E-40
320	5.12E-21	1.50E-20	6.90E+00	5.31E-40	8.48E-21	9.07E-21	6.90E+00	5.31E-40	2.98E-20	2.58E-21	6.90E+00	5.31E-40

Table S6: Bimolecular rate constant  $k_b$  in ( $\text{cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$ ) for  $\text{H}_2\text{O}$  catalyzed channels for OAT path for  $\text{CH}_2\text{OO} + \text{cis/trans-HONO}$  within temperature range 213-320K.

cis-HONO				trans-HONO			
Temp (K)	Path A	Path B	Path C	Temp (K)	Path A	Path B	Path C
213	6.62E-30	1.39E-28	2.51E-29	213	1.78E-22	3.55E-18	2.52E-21
216	1.09E-29	2.15E-28	4.01E-29	216	2.29E-22	3.59E-18	3.02E-21
219	1.77E-29	3.27E-28	6.33E-29	219	2.93E-22	3.62E-18	3.62E-21
224	3.90E-29	6.47E-28	1.33E-28	224	4.37E-22	3.70E-18	4.85E-21
235	1.97E-28	2.63E-27	6.07E-28	235	9.93E-22	3.86E-18	8.86E-21
250	1.46E-27	1.50E-26	3.99E-27	250	2.76E-21	4.15E-18	1.89E-20
259	4.36E-27	3.89E-26	1.12E-26	259	4.81E-21	4.30E-18	2.86E-20
265	8.73E-27	7.11E-26	2.16E-26	265	6.85E-21	4.42E-18	3.72E-20
278	3.57E-26	2.43E-25	8.18E-26	278	1.41E-20	4.70E-18	6.39E-20
280	4.40E-26	2.91E-25	9.98E-26	280	1.56E-20	4.74E-18	6.92E-20
290	1.18E-25	6.89E-25	2.53E-25	290	2.59E-20	4.95E-18	1.01E-19
298	2.49E-25	1.33E-24	5.16E-25	298	3.81E-20	5.14E-18	1.35E-19
300	2.98E-25	1.55E-24	6.11E-25	300	4.19E-20	5.19E-18	1.46E-19
310	7.14E-25	3.33E-24	1.40E-24	310	6.55E-20	5.42E-18	2.04E-19
320	1.63E-24	6.86E-24	3.06E-24	320	1.00E-19	5.68E-18	2.82E-19

Table S7: Bimolecular rate constant  $k_b$  in ( $\text{cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$ ) for  $(\text{H}_2\text{O})_2$  catalyzed channels for OAT path for  $\text{CH}_2\text{OO} + \text{cis/trans-HONO}$  within temperature range 213-320K.

cis-HONO				trans-HONO			
Temp (K)	Path A	Path B	Path C	Temp (K)	Path A	Path B	Path C
213	1.86E-25	2.91E-26	4.74E-28	213	7.54E-21	3.16E-21	7.18E-23
216	2.46E-25	4.12E-26	7.32E-28	216	8.33E-21	3.54E-21	8.90E-23
219	3.22E-25	5.78E-26	1.11E-27	219	9.19E-21	3.96E-21	1.10E-22
224	5.04E-25	1.01E-25	2.22E-27	224	1.08E-20	4.75E-21	1.55E-22
235	1.26E-24	3.13E-25	9.07E-27	235	1.50E-20	6.93E-21	3.15E-22
250	3.90E-24	1.28E-24	5.19E-26	250	2.28E-20	1.11E-20	7.60E-22
259	7.27E-24	2.77E-24	1.35E-25	259	2.88E-20	1.45E-20	1.24E-21
265	1.08E-23	4.54E-24	2.49E-25	265	3.33E-20	1.71E-20	1.68E-21
278	2.41E-23	1.23E-23	8.56E-25	278	4.49E-20	2.41E-20	3.16E-21
280	2.72E-23	1.43E-23	1.03E-24	280	4.71E-20	2.54E-20	3.47E-21
290	4.78E-23	2.88E-23	2.45E-24	290	5.83E-20	3.24E-20	5.42E-21
298	7.34E-23	4.90E-23	4.73E-24	298	6.85E-20	3.90E-20	7.59E-21
300	8.14E-23	5.57E-23	5.54E-24	300	7.11E-20	4.07E-20	8.21E-21
310	1.34E-22	1.04E-22	1.20E-23	310	8.64E-20	5.08E-20	1.22E-20
320	2.16E-22	1.87E-22	2.47E-23	320	1.04E-19	6.26E-20	1.78E-20

Table S8: Termolecular rate constant  $k_t$  in ( $\text{cm}^6 \text{ molecule}^{-2} \text{ sec}^{-1}$ ) for  $\text{H}_2\text{O}$  catalyzed channels for SHAT-WM for  $\text{CH}_2\text{OO} + \text{cis-HONO}$  within temperature range 213-320K.

Temp (K)	PATH A				PATH B				PATH C			
	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt
213	1.66E-18	1.8E-19	2.77E+03	8.28E-34	7.88E-20	3.791E-18	2.77E+03	8.28E-34	4.38E-19	6.828E-19	2.77E+03	8.28E-34
216	1.28E-18	1.415E-19	3.65E+03	6.59E-34	6.48E-20	2.786E-18	3.65E+03	6.59E-34	3.47E-19	5.203E-19	3.65E+03	6.59E-34
219	9.88E-19	1.121E-19	4.78E+03	5.29E-34	5.36E-20	2.065E-18	4.78E+03	5.29E-34	2.77E-19	3.996E-19	4.78E+03	5.29E-34
224	6.55E-19	7.705E-20	7.37E+03	3.72E-34	3.95E-20	1.277E-18	7.37E+03	3.72E-34	1.93E-19	2.618E-19	7.37E+03	3.72E-34
235	2.83E-19	3.585E-20	1.80E+04	1.82E-34	2.12E-20	4.787E-19	1.80E+04	1.82E-34	9.20E-20	1.104E-19	1.80E+04	1.82E-34
250	1.03E-19	1.415E-20	5.36E+04	7.77E-35	9.99E-21	1.453E-19	5.36E+04	7.77E-35	3.74E-20	3.877E-20	5.36E+04	7.77E-35
259	5.92E-20	8.557E-21	9.72E+04	4.92E-35	6.65E-21	7.619E-20	9.72E+04	4.92E-35	2.30E-20	2.203E-20	9.72E+04	4.92E-35
265	4.20E-20	6.243E-21	1.42E+05	3.71E-35	5.15E-21	5.084E-20	1.42E+05	3.71E-35	1.69E-20	1.546E-20	1.42E+05	3.71E-35
278	2.10E-20	3.315E-21	3.02E+05	2.11E-35	3.09E-21	2.255E-20	3.02E+05	2.11E-35	9.17E-21	7.6E-21	3.02E+05	2.11E-35
280	1.90E-20	3.024E-21	3.38E+05	1.94E-35	2.87E-21	2.004E-20	3.38E+05	1.94E-35	8.39E-21	6.857E-21	3.38E+05	1.94E-35
290	1.18E-20	1.95E-21	5.75E+05	1.32E-35	2.02E-21	1.14E-20	5.75E+05	1.32E-35	5.48E-21	4.195E-21	5.75E+05	1.32E-35
298	8.25E-21	1.405E-21	8.58E+05	9.94E-36	1.55E-21	7.478E-21	8.58E+05	9.94E-36	3.99E-21	2.906E-21	8.58E+05	9.94E-36
300	7.57E-21	1.298E-21	9.45E+05	9.28E-36	1.45E-21	6.755E-21	9.45E+05	9.28E-36	3.69E-21	2.66E-21	9.45E+05	9.28E-36
310	5.01E-21	8.887E-22	1.50E+06	6.70E-36	1.07E-21	4.149E-21	1.50E+06	6.70E-36	2.56E-21	1.741E-21	1.50E+06	6.70E-36
320	3.41E-21	6.244E-22	2.33E+06	4.96E-36	8.09E-22	2.634E-21	2.33E+06	4.96E-36	1.82E-21	1.174E-21	2.33E+06	4.96E-36



Table S9: Termolecular rate constant  $k_t$  in ( $\text{cm}^6 \text{ molecule}^{-2} \text{ sec}^{-1}$ ) for  $\text{H}_2\text{O}$  catalyzed channels for SHAT-WM for  $\text{CH}_2\text{OO} + \text{trans-HONO}$  within temperature range 213-320K.

Temp (K)	PATH A				PATH B				PATH C			
	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt
213	6.186E-18	6.674E-18	9.04E+02	3.73E-32	3.10E-22	1.33E-13	9.04E+02	3.73E-32	4.38E-19	9.433E-17	9.04E+02	3.73E-32
216	4.579E-18	5.106E-18	1.22E+03	2.85E-32	2.93E-22	7.988E-14	1.22E+03	2.85E-32	3.47E-19	6.738E-17	1.22E+03	2.85E-32
219	3.418E-18	3.937E-18	1.63E+03	2.19E-32	2.77E-22	4.866E-14	1.63E+03	2.19E-32	2.77E-19	4.86E-17	1.63E+03	2.19E-32
224	2.139E-18	2.593E-18	2.60E+03	1.44E-32	2.53E-22	2.194E-14	2.60E+03	1.44E-32	1.93E-19	2.877E-17	2.60E+03	1.44E-32
235	8.209E-19	1.105E-18	6.80E+03	6.17E-33	2.11E-22	4.297E-15	6.80E+03	6.17E-33	9.20E-20	9.859E-18	6.80E+03	6.17E-33
250	2.565E-19	3.916E-19	2.20E+04	2.21E-33	1.71E-22	5.884E-16	2.20E+04	2.21E-33	3.74E-20	2.685E-18	2.20E+04	2.21E-33
259	1.366E-19	2.233E-19	4.17E+04	1.27E-33	1.53E-22	1.998E-16	4.17E+04	1.27E-33	2.30E-20	1.328E-18	4.17E+04	1.27E-33
265	9.207E-20	1.571E-19	6.24E+04	9.03E-34	1.43E-22	1.014E-16	6.24E+04	9.03E-34	1.69E-20	8.538E-19	6.24E+04	9.03E-34
278	4.165E-20	7.743E-20	1.41E+05	4.54E-34	1.25E-22	2.583E-17	1.41E+05	4.54E-34	9.17E-21	3.517E-19	1.41E+05	4.54E-34
280	3.712E-20	6.988E-20	1.58E+05	4.11E-34	1.23E-22	2.117E-17	1.58E+05	4.11E-34	8.39E-21	3.092E-19	1.58E+05	4.11E-34
290	2.141E-20	4.279E-20	2.79E+05	2.56E-34	1.12E-22	8.172E-18	2.79E+05	2.56E-34	5.48E-21	1.671E-19	2.79E+05	2.56E-34
298	1.419E-20	2.965E-20	4.28E+05	1.80E-34	1.05E-22	4.001E-18	4.28E+05	1.80E-34	3.99E-21	1.055E-19	4.28E+05	1.80E-34
300	1.285E-20	2.714E-20	4.74E+05	1.65E-34	1.04E-22	3.367E-18	4.74E+05	1.65E-34	3.69E-21	9.438E-20	4.74E+05	1.65E-34
310	7.982E-21	1.777E-20	7.79E+05	1.10E-34	9.64E-23	1.471E-18	7.79E+05	1.10E-34	2.56E-21	5.544E-20	7.79E+05	1.10E-34
320	5.121E-21	1.197E-20	1.24E+06	7.60E-35	9.04E-23	6.781E-19	1.24E+06	7.59E-35	1.82E-21	3.375E-20	1.24E+06	7.60E-35

Table S10: Termolecular rate constant  $k_t$  in ( $\text{cm}^6 \text{ molecule}^{-2} \text{ sec}^{-1}$ ) for  $\text{H}_2\text{O}$  catalyzed channels for DHAT-WM for  $\text{CH}_2\text{OO} + \text{cis-HONO}$  within temperature range 213-320K.

Temp (K)	PATH A				PATH B				PATH C			
	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt
213	1.66E-18	1.35E-17	3.48E+07	7.78E-28	7.88E-20	2.84E-16	3.48E+07	7.78E-28	4.38E-19	5.11E-17	3.48E+07	7.78E-28
216	1.28E-18	1.02E-17	3.80E+07	4.93E-28	6.48E-20	2.00E-16	3.80E+07	4.92E-28	3.47E-19	3.74E-17	3.80E+07	4.93E-28
219	9.88E-19	7.73E-18	4.10E+07	3.13E-28	5.36E-20	1.43E-16	4.10E+07	3.13E-28	2.77E-19	2.76E-17	4.10E+07	3.13E-28
224	6.55E-19	4.99E-18	4.70E+07	1.54E-28	3.95E-20	8.27E-17	4.70E+07	1.54E-28	1.93E-19	1.70E-17	4.70E+07	1.54E-28
235	2.83E-19	2.03E-18	6.20E+07	3.57E-29	2.12E-20	2.72E-17	6.20E+07	3.57E-29	9.20E-20	6.26E-18	6.20E+07	3.57E-29
250	1.03E-19	6.81E-19	8.73E+07	6.10E-30	9.99E-21	6.99E-18	8.73E+07	6.10E-30	3.74E-20	1.87E-18	8.73E+07	6.10E-30
259	5.92E-20	3.76E-19	1.05E+08	2.35E-30	6.65E-21	3.35E-18	1.05E+08	2.35E-30	2.30E-20	9.69E-19	1.05E+08	2.35E-30
265	4.20E-20	2.59E-19	1.19E+08	1.29E-30	5.15E-21	2.11E-18	1.19E+08	1.29E-30	1.69E-20	6.42E-19	1.19E+08	1.29E-30
278	2.10E-20	1.23E-19	1.51E+08	3.89E-31	3.09E-21	8.33E-19	1.51E+08	3.89E-31	9.17E-21	2.81E-19	1.51E+08	3.89E-31
280	1.90E-20	1.10E-19	1.57E+08	3.27E-31	2.87E-21	7.28E-19	1.57E+08	3.27E-31	8.39E-21	2.49E-19	1.57E+08	3.27E-31
290	1.18E-20	6.53E-20	1.85E+08	1.43E-31	2.02E-21	3.82E-19	1.85E+08	1.43E-31	5.48E-21	1.40E-19	1.85E+08	1.43E-31
298	8.25E-21	4.42E-20	2.11E+08	7.68E-32	1.55E-21	2.35E-19	2.11E+08	7.68E-32	3.99E-21	9.13E-20	2.11E+08	7.68E-32
300	7.57E-21	4.02E-20	2.18E+08	6.63E-32	1.45E-21	2.09E-19	2.18E+08	6.63E-32	3.69E-21	8.24E-20	2.18E+08	6.63E-32
310	5.01E-21	2.56E-20	2.52E+08	3.22E-32	1.07E-21	1.19E-19	2.52E+08	3.23E-32	2.56E-21	5.01E-20	2.52E+08	3.22E-32
320	3.41E-21	1.68E-20	2.90E+08	1.66E-32	8.09E-22	7.07E-20	2.90E+08	1.66E-32	1.82E-21	3.15E-20	2.90E+08	1.66E-32

Table S11: Termolecular rate constant  $k_t$  in ( $\text{cm}^6 \text{ molecule}^{-2} \text{ sec}^{-1}$ ) for  $\text{H}_2\text{O}$  catalyzed channels for DHAT-WM for  $\text{CH}_2\text{OO} + \text{trans-HONO}$  within temperature range 213-320K.

Temp (K)	PATH A				PATH B				PATH C			
	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt
213	6.186E-18	1.047E-17	7.88E+07	5.10E-27	3.10E-22	2.09E-13	7.88E+07	5.10E-27	4.38E-19	1.48E-16	7.88E+07	5.10E-27
216	4.579E-18	7.965E-18	8.57E+07	3.13E-27	2.93E-22	1.25E-13	8.57E+07	3.13E-27	3.47E-19	1.05E-16	8.57E+07	3.13E-27
219	3.418E-18	6.107E-18	9.31E+07	1.94E-27	2.77E-22	7.55E-14	9.31E+07	1.94E-27	2.77E-19	7.54E-17	9.31E+07	1.94E-27
224	2.139E-18	3.986E-18	1.06E+08	9.06E-28	2.53E-22	3.37E-14	1.06E+08	9.07E-28	1.93E-19	4.42E-17	1.06E+08	9.06E-28
235	8.209E-19	1.665E-18	1.40E+08	1.91E-28	2.11E-22	6.48E-15	1.40E+08	1.91E-28	9.20E-20	1.49E-17	1.40E+08	1.91E-28
250	2.565E-19	5.754E-19	1.95E+08	2.88E-29	1.71E-22	8.65E-16	1.95E+08	2.88E-29	3.74E-20	3.95E-18	1.95E+08	2.88E-29
259	1.366E-19	3.233E-19	2.34E+08	1.03E-29	1.53E-22	2.89E-16	2.34E+08	1.03E-29	2.30E-20	1.92E-18	2.34E+08	1.03E-29
265	9.207E-20	2.252E-19	2.62E+08	5.44E-30	1.43E-22	1.45E-16	2.62E+08	5.44E-30	1.69E-20	1.22E-18	2.62E+08	5.44E-30
278	4.165E-20	1.088E-19	3.30E+08	1.50E-30	1.25E-22	3.63E-17	3.30E+08	1.50E-30	9.17E-21	4.94E-19	3.30E+08	1.50E-30
280	3.712E-20	9.786E-20	3.42E+08	1.24E-30	1.23E-22	2.97E-17	3.42E+08	1.24E-30	8.39E-21	4.33E-19	3.42E+08	1.24E-30
290	2.141E-20	5.903E-20	4.01E+08	5.07E-31	1.12E-22	1.13E-17	4.01E+08	5.07E-31	5.48E-21	2.31E-19	4.01E+08	5.07E-31
298	1.419E-20	4.042E-20	4.53E+08	2.60E-31	1.05E-22	5.45E-18	4.53E+08	2.60E-31	3.99E-21	1.44E-19	4.53E+08	2.60E-31
300	1.285E-20	3.689E-20	4.67E+08	2.21E-31	1.04E-22	4.58E-18	4.67E+08	2.21E-31	3.69E-21	1.28E-19	4.67E+08	2.21E-31
310	7.982E-21	2.381E-20	5.37E+08	1.02E-31	9.64E-23	1.97E-18	5.37E+08	1.02E-31	2.56E-21	7.43E-20	5.37E+08	1.02E-31
320	5.121E-21	1.582E-20	6.13E+08	4.96E-32	9.04E-23	8.96E-19	6.13E+08	4.96E-32	1.82E-21	4.46E-20	6.13E+08	4.96E-32

Table S12: Bimolecular rate constant  $k_b$  in ( $\text{cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$ ) for  $\text{H}_2\text{O}$  catalyzed channels for SHAT-WM path for  $\text{CH}_2\text{OO} + \text{cis/trans-HONO}$  within temperature range 213-320K.

cis-HONO				trans-HONO			
Temp (K)	Path A	Path B	Path C	Temp (K)	Path A	Path B	Path C
213	4.98E-16	1.05E-14	1.89E-15	213	6.03E-15	1.20E-10	8.53E-14
216	5.17E-16	1.02E-14	1.90E-15	216	6.22E-15	9.74E-11	8.21E-14
219	5.36E-16	9.87E-15	1.91E-15	219	6.42E-15	7.93E-11	7.93E-14
224	5.68E-16	9.42E-15	1.93E-15	224	6.75E-15	5.71E-11	7.49E-14
235	6.44E-16	8.60E-15	1.98E-15	235	7.52E-15	2.92E-11	6.71E-14
250	7.58E-16	7.78E-15	2.08E-15	250	8.62E-15	1.30E-11	5.91E-14
259	8.32E-16	7.41E-15	2.14E-15	259	9.32E-15	8.34E-12	5.54E-14
265	8.84E-16	7.20E-15	2.19E-15	265	9.81E-15	6.33E-12	5.33E-14
278	1.00E-15	6.82E-15	2.30E-15	278	1.09E-14	3.63E-12	4.95E-14
280	1.02E-15	6.77E-15	2.32E-15	280	1.11E-14	3.35E-12	4.90E-14
290	1.12E-15	6.55E-15	2.41E-15	290	1.20E-14	2.28E-12	4.67E-14
298	1.20E-15	6.41E-15	2.49E-15	298	1.27E-14	1.71E-12	4.51E-14
300	1.23E-15	6.38E-15	2.51E-15	300	1.29E-14	1.60E-12	4.48E-14
310	1.34E-15	6.24E-15	2.62E-15	310	1.38E-14	1.15E-12	4.32E-14
320	1.45E-15	6.13E-15	2.73E-15	320	1.48E-14	8.40E-13	4.18E-14

Table S13: Bimolecular rate constant  $k_b$  in ( $\text{cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$ ) for  $\text{H}_2\text{O}$  catalyzed channels for DHAT-WM path for  $\text{CH}_2\text{OO} + \text{cis/trans-HONO}$  within temperature range 213-320K.

cis-HONO				trans-HONO			
Temp (K)	Path A	Path B	Path C	Temp (K)	Path A	Path B	Path C
213	4.68E-10	9.86E-09	1.78E-09	213	8.25E-10	1.64E-05	1.17E-08
216	3.86E-10	7.60E-09	1.42E-09	216	6.83E-10	1.07E-05	9.01E-09
219	3.17E-10	5.84E-09	1.13E-09	219	5.68E-10	7.03E-06	7.02E-09
224	2.34E-10	3.89E-09	7.97E-10	224	4.24E-10	3.59E-06	4.70E-09
235	1.26E-10	1.68E-09	3.88E-10	235	2.32E-10	9.04E-07	2.07E-09
250	5.95E-11	6.11E-10	1.63E-10	250	1.12E-10	1.69E-07	7.69E-10
259	3.96E-11	3.53E-10	1.02E-10	259	7.56E-11	6.76E-08	4.49E-10
265	3.08E-11	2.51E-10	7.63E-11	265	5.90E-11	3.81E-08	3.21E-10
278	1.85E-11	1.26E-10	4.24E-11	278	3.59E-11	1.20E-08	1.63E-10
280	1.72E-11	1.14E-10	3.90E-11	280	3.34E-11	1.01E-08	1.48E-10
290	1.21E-11	7.07E-11	2.60E-11	290	2.37E-11	4.52E-09	9.25E-11
298	9.31E-12	4.96E-11	1.93E-11	298	1.83E-11	2.47E-09	6.52E-11
300	8.76E-12	4.56E-11	1.80E-11	300	1.72E-11	2.14E-09	5.99E-11
310	6.43E-12	3.00E-11	1.26E-11	310	1.28E-11	1.06E-09	3.99E-11
320	4.86E-12	2.05E-11	9.14E-12	320	9.69E-12	5.49E-10	2.73E-11

Table S14: Termolecular rate constant  $k_t$  in ( $\text{cm}^6 \text{ molecule}^{-2} \text{ sec}^{-1}$ ) for  $(\text{H}_2\text{O})_2$  catalyzed channels for SHAT-WD for  $\text{CH}_2\text{OO} + \text{cis-HONO}$  within temperature range 213-320K.

Temp (K)	PATH A				PATH B				PATH C			
	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt
213	1.661E-18	2.658E-16	1.72E+02	7.57E-32	1.06E-17	4.166E-17	1.72E+02	7.58E-32	6.499E-16	6.792E-19	1.72E+02	7.57E-32
216	1.276E-18	1.748E-16	2.33E+02	5.19E-32	7.602E-18	2.933E-17	2.33E+02	5.19E-32	4.284E-16	5.205E-19	2.33E+02	5.19E-32
219	9.875E-19	1.163E-16	3.14E+02	3.60E-32	5.505E-18	2.086E-17	3.14E+02	3.60E-32	2.857E-16	4.019E-19	3.14E+02	3.60E-32
224	6.549E-19	6.041E-17	5.06E+02	2.00E-32	3.279E-18	1.207E-17	5.06E+02	2.00E-32	1.49E-16	2.656E-19	5.06E+02	2.00E-32
235	2.833E-19	1.58E-17	1.36E+03	6.07E-33	1.136E-18	3.942E-18	1.36E+03	6.08E-33	3.923E-17	1.141E-19	1.36E+03	6.07E-33
250	1.025E-19	3.08E-18	4.55E+03	1.43E-33	3.123E-19	1.011E-18	4.55E+03	1.44E-33	7.698E-18	4.102E-20	4.55E+03	1.44E-33
259	5.918E-20	1.267E-18	8.80E+03	6.60E-34	1.55E-19	4.838E-19	8.80E+03	6.60E-34	3.175E-18	2.361E-20	8.80E+03	6.60E-34
265	4.195E-20	7.251E-19	1.33E+04	4.06E-34	9.985E-20	3.046E-19	1.33E+04	4.06E-34	1.82E-18	1.671E-20	1.33E+04	4.06E-34
278	2.103E-20	2.356E-19	3.10E+04	1.53E-34	4.121E-20	1.202E-19	3.10E+04	1.53E-34	5.926E-19	8.359E-21	3.10E+04	1.53E-34
280	1.902E-20	2E-19	3.50E+04	1.33E-34	3.624E-20	1.05E-19	3.50E+04	1.33E-34	5.034E-19	7.561E-21	3.50E+04	1.33E-34
290	1.18E-20	9.147E-20	6.32E+04	6.82E-35	1.959E-20	5.506E-20	6.32E+04	6.81E-35	2.304E-19	4.683E-21	6.32E+04	6.82E-35
298	8.251E-21	5.086E-20	9.85E+04	4.13E-35	1.236E-20	3.395E-20	9.85E+04	4.13E-35	1.281E-19	3.275E-21	9.85E+04	4.13E-35
300	7.57E-21	4.414E-20	1.10E+05	3.66E-35	1.106E-20	3.022E-20	1.10E+05	3.67E-35	1.112E-19	3.005E-21	1.10E+05	3.66E-35
310	5.012E-21	2.236E-20	1.84E+05	2.06E-35	6.486E-21	1.728E-20	1.84E+05	2.06E-35	5.631E-20	1.99E-21	1.84E+05	2.06E-35
320	3.413E-21	1.183E-20	2.99E+05	1.21E-35	3.94E-21	1.025E-20	2.99E+05	1.21E-35	2.979E-20	1.356E-21	2.99E+05	1.21E-35

Table S15: Termolecular rate constant  $k_t$  in ( $\text{cm}^6 \text{ molecule}^{-2} \text{ sec}^{-1}$ ) for  $(\text{H}_2\text{O})_2$  catalyzed channels for SHAT-WD for  $\text{CH}_2\text{OO}$  + trans-HONO within temperature range 213-320K.

Temp (K)	PATH A					PATH B					PATH C					
	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt
213	6.186E-18	2.841E-17	1.48E+03	2.61E-31	1.476E-17	1.19E-17	1.48E+03	2.61E-31	6.499E-16	2.704E-19	1.48E+03	2.61E-31	6.499E-16	2.704E-19	1.48E+03	2.61E-31
216	4.579E-18	1.937E-17	2.00E+03	1.77E-31	1.078E-17	8.228E-18	2.00E+03	1.77E-31	4.284E-16	2.07E-19	2.00E+03	1.77E-31	4.284E-16	2.07E-19	2.00E+03	1.77E-31
219	3.418E-18	1.335E-17	2.67E+03	1.22E-31	7.941E-18	5.745E-18	2.67E+03	1.22E-31	2.857E-16	1.597E-19	2.67E+03	1.22E-31	2.857E-16	1.597E-19	2.67E+03	1.22E-31
224	2.139E-18	7.337E-18	4.27E+03	6.70E-32	4.863E-18	3.227E-18	4.27E+03	6.70E-32	1.49E-16	1.053E-19	4.27E+03	6.70E-32	1.49E-16	1.053E-19	4.27E+03	6.70E-32
235	8.209E-19	2.153E-18	1.12E+04	1.98E-32	1.784E-18	9.91E-19	1.12E+04	1.98E-32	3.923E-17	4.505E-20	1.12E+04	1.98E-32	3.923E-17	4.505E-20	1.12E+04	1.98E-32
250	2.565E-19	4.822E-19	3.68E+04	4.55E-33	5.262E-19	2.351E-19	3.68E+04	4.55E-33	7.698E-18	1.607E-20	3.68E+04	4.55E-33	7.698E-18	1.607E-20	3.68E+04	4.55E-33
259	1.366E-19	2.138E-19	7.05E+04	2.06E-33	2.714E-19	1.076E-19	7.05E+04	2.06E-33	3.175E-18	9.198E-21	7.05E+04	2.06E-33	3.175E-18	9.198E-21	7.05E+04	2.06E-33
265	9.207E-20	1.282E-19	1.06E+05	1.26E-33	1.792E-19	6.589E-20	1.06E+05	1.26E-33	1.82E-18	6.485E-21	1.06E+05	1.26E-33	1.82E-18	6.485E-21	1.06E+05	1.26E-33
278	4.165E-20	4.575E-20	2.45E+05	4.66E-34	7.767E-20	2.453E-20	2.45E+05	4.66E-34	5.926E-19	3.215E-21	2.45E+05	4.66E-34	5.926E-19	3.215E-21	2.45E+05	4.66E-34
280	3.712E-20	3.938E-20	2.76E+05	4.04E-34	6.88E-20	2.125E-20	2.76E+05	4.04E-34	5.034E-19	2.904E-21	2.76E+05	4.04E-34	5.034E-19	2.904E-21	2.76E+05	4.04E-34
290	2.141E-20	1.921E-20	4.95E+05	2.04E-34	3.85E-20	1.068E-20	4.95E+05	2.04E-34	2.304E-19	1.786E-21	4.95E+05	2.04E-34	2.304E-19	1.786E-21	4.95E+05	2.04E-34
298	1.419E-20	1.121E-20	7.70E+05	1.22E-34	2.492E-20	6.381E-21	7.70E+05	1.22E-34	1.281E-19	1.241E-21	7.70E+05	1.22E-34	1.281E-19	1.241E-21	7.70E+05	1.22E-34
300	1.285E-20	9.843E-21	8.56E+05	1.08E-34	2.244E-20	5.634E-21	8.56E+05	1.08E-34	1.112E-19	1.137E-21	8.56E+05	1.08E-34	1.112E-19	1.137E-21	8.56E+05	1.08E-34
310	7.982E-21	5.271E-21	1.43E+06	6.02E-35	1.357E-20	3.101E-21	1.43E+06	6.02E-35	5.631E-20	7.472E-22	1.43E+06	6.02E-35	5.631E-20	7.472E-22	1.43E+06	6.02E-35
320	5.121E-21	2.939E-21	2.32E+06	3.49E-35	8.483E-21	1.774E-21	2.32E+06	3.49E-35	2.979E-20	5.051E-22	2.32E+06	3.49E-35	2.979E-20	5.051E-22	2.32E+06	3.49E-35

Table S16: Termolecular rate constant  $k_t$  in ( $\text{cm}^6 \text{ molecule}^{-2} \text{ sec}^{-1}$ ) for  $(\text{H}_2\text{O})_2$  catalyzed channels for THAT-WD for  $\text{CH}_2\text{OO} + \text{cis-HONO}$  within temperature range 213-320K.

Temp (K)	PATH A				PATH B				PATH C			
	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt
213	1.66E-18	3.32E-15	8.27E+07	4.55E-25	1.06E-17	5.20E-16	8.27E+07	4.56E-25	6.50E-16	8.48E-18	8.27E+07	4.55E-25
216	1.28E-18	2.12E-15	8.98E+07	2.43E-25	7.60E-18	3.56E-16	8.98E+07	2.43E-25	4.28E-16	6.31E-18	8.98E+07	2.43E-25
219	9.88E-19	1.37E-15	9.73E+07	1.32E-25	5.51E-18	2.46E-16	9.73E+07	1.32E-25	2.86E-16	4.74E-18	9.73E+07	1.32E-25
224	6.55E-19	6.82E-16	1.11E+08	4.94E-26	3.28E-18	1.36E-16	1.11E+08	4.94E-26	1.49E-16	3.00E-18	1.11E+08	4.94E-26
235	2.83E-19	1.62E-16	1.44E+08	6.64E-27	1.14E-18	4.05E-17	1.44E+08	6.64E-27	3.92E-17	1.17E-18	1.44E+08	6.64E-27
250	1.03E-19	2.82E-17	1.99E+08	5.75E-28	3.12E-19	9.25E-18	1.99E+08	5.75E-28	7.70E-18	3.75E-19	1.99E+08	5.75E-28
259	5.92E-20	1.09E-17	2.37E+08	1.52E-28	1.55E-19	4.15E-18	2.37E+08	1.52E-28	3.18E-18	2.02E-19	2.37E+08	1.52E-28
265	4.20E-20	5.96E-18	2.64E+08	6.61E-29	9.99E-20	2.51E-18	2.64E+08	6.61E-29	1.82E-18	1.37E-19	2.64E+08	6.61E-29
278	2.10E-20	1.78E-18	3.30E+08	1.23E-29	4.12E-20	9.08E-19	3.30E+08	1.23E-29	5.93E-19	6.31E-20	3.30E+08	1.23E-29
280	1.90E-20	1.49E-18	3.40E+08	9.66E-30	3.62E-20	7.83E-19	3.40E+08	9.66E-30	5.03E-19	5.64E-20	3.40E+08	9.66E-30
290	1.18E-20	6.42E-19	3.97E+08	3.01E-30	1.96E-20	3.86E-19	3.97E+08	3.00E-30	2.30E-19	3.29E-20	3.97E+08	3.00E-30
298	8.25E-21	3.41E-19	4.45E+08	1.25E-30	1.24E-20	2.28E-19	4.45E+08	1.25E-30	1.28E-19	2.19E-20	4.45E+08	1.25E-30
300	7.57E-21	2.92E-19	4.57E+08	1.01E-30	1.11E-20	2.00E-19	4.57E+08	1.01E-30	1.11E-19	1.99E-20	4.57E+08	1.01E-30
310	5.01E-21	1.40E-19	5.22E+08	3.67E-31	6.49E-21	1.08E-19	5.22E+08	3.67E-31	5.63E-20	1.25E-20	5.22E+08	3.67E-31
320	3.41E-21	7.05E-20	5.91E+08	1.42E-31	3.94E-21	6.10E-20	5.91E+08	1.42E-31	2.98E-20	8.07E-21	5.91E+08	1.42E-31



Table S17: Termolecular rate constant  $k_t$  in ( $\text{cm}^6 \text{ molecule}^{-2} \text{ sec}^{-1}$ ) for  $(\text{H}_2\text{O})_2$  catalyzed channels for THAT-WD for  $\text{CH}_2\text{OO} + \text{trans-HONO}$  within temperature range 213-320K.

Temp (K)	PATH A				PATH B				PATH C			
	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt
213	6.19E-18	6.11E-14	7.63E+06	2.89E-24	1.48E-17	2.56E-14	7.63E+06	2.88E-24	6.50E-16	5.82E-16	7.63E+06	2.88E-24
216	4.58E-18	3.82E-14	8.55E+06	1.50E-24	1.08E-17	1.62E-14	8.55E+06	1.50E-24	4.28E-16	4.09E-16	8.55E+06	1.50E-24
219	3.42E-18	2.42E-14	9.54E+06	7.90E-25	7.94E-18	1.04E-14	9.54E+06	7.90E-25	2.86E-16	2.90E-16	9.54E+06	7.90E-25
224	2.14E-18	1.16E-14	1.14E+07	2.84E-25	4.86E-18	5.12E-15	1.14E+07	2.84E-25	1.49E-16	1.67E-16	1.14E+07	2.84E-25
235	8.21E-19	2.59E-15	1.64E+07	3.48E-26	1.78E-18	1.19E-15	1.64E+07	3.49E-26	3.92E-17	5.41E-17	1.64E+07	3.48E-26
250	2.57E-19	4.12E-16	2.56E+07	2.71E-27	5.26E-19	2.01E-16	2.56E+07	2.71E-27	7.70E-18	1.37E-17	2.56E+07	2.71E-27
259	1.37E-19	1.52E-16	3.26E+07	6.77E-28	2.71E-19	7.64E-17	3.26E+07	6.77E-28	3.18E-18	6.53E-18	3.26E+07	6.77E-28
265	9.21E-20	8.10E-17	3.80E+07	2.83E-28	1.79E-19	4.16E-17	3.80E+07	2.84E-28	1.82E-18	4.10E-18	3.80E+07	2.84E-28
278	4.17E-20	2.28E-17	5.17E+07	4.91E-29	7.77E-20	1.22E-17	5.17E+07	4.91E-29	5.93E-19	1.60E-18	5.17E+07	4.91E-29
280	3.71E-20	1.90E-17	5.40E+07	3.81E-29	6.88E-20	1.02E-17	5.40E+07	3.80E-29	5.03E-19	1.40E-18	5.40E+07	3.81E-29
290	2.14E-20	7.84E-18	6.69E+07	1.12E-29	3.85E-20	4.36E-18	6.69E+07	1.12E-29	2.30E-19	7.29E-19	6.69E+07	1.12E-29
298	1.42E-20	4.04E-18	7.86E+07	4.50E-30	2.49E-20	2.30E-18	7.86E+07	4.50E-30	1.28E-19	4.47E-19	7.86E+07	4.50E-30
300	1.29E-20	3.44E-18	8.17E+07	3.61E-30	2.24E-20	1.97E-18	8.17E+07	3.61E-30	1.11E-19	3.97E-19	8.17E+07	3.61E-30
310	7.98E-21	1.59E-18	9.83E+07	1.25E-30	1.36E-20	9.37E-19	9.83E+07	1.25E-30	5.63E-20	2.26E-19	9.83E+07	1.25E-30
320	5.12E-21	7.75E-19	1.17E+08	4.64E-31	8.48E-21	4.68E-19	1.17E+08	4.64E-31	2.98E-20	1.33E-19	1.17E+08	4.64E-31

Table S18: Bimolecular rate constant  $k_b$  in ( $\text{cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$ ) for  $(\text{H}_2\text{O})_2$  catalyzed channels for SHAT-WD path for  $\text{CH}_2\text{OO} + \text{cis/trans-HONO}$  within temperature range 213-320K.

cis-HONO				trans-HONO			
Temp (K)	Path A	Path B	Path C	Temp (K)	Path A	Path B	Path C
213	4.56E-14	7.15E-15	1.17E-16	213	4.21E-14	1.77E-14	4.01E-16
216	4.07E-14	6.83E-15	1.21E-16	216	3.87E-14	1.64E-14	4.14E-16
219	3.65E-14	6.54E-15	1.26E-16	219	3.57E-14	1.54E-14	4.27E-16
224	3.06E-14	6.11E-15	1.35E-16	224	3.13E-14	1.38E-14	4.49E-16
235	2.14E-14	5.35E-15	1.55E-16	235	2.41E-14	1.11E-14	5.05E-16
250	1.40E-14	4.60E-15	1.86E-16	250	1.77E-14	8.65E-15	5.91E-16
259	1.11E-14	4.26E-15	2.08E-16	259	1.51E-14	7.59E-15	6.49E-16
265	9.67E-15	4.06E-15	2.23E-16	265	1.36E-14	7.01E-15	6.90E-16
278	7.30E-15	3.72E-15	2.59E-16	278	1.12E-14	6.00E-15	7.86E-16
280	7.01E-15	3.68E-15	2.65E-16	280	1.09E-14	5.87E-15	8.02E-16
290	5.78E-15	3.48E-15	2.96E-16	290	9.52E-15	5.29E-15	8.85E-16
298	5.01E-15	3.34E-15	3.23E-16	298	8.63E-15	4.91E-15	9.55E-16
300	4.84E-15	3.31E-15	3.30E-16	300	8.43E-15	4.83E-15	9.74E-16
310	4.11E-15	3.18E-15	3.66E-16	310	7.54E-15	4.44E-15	1.07E-15
320	3.54E-15	3.06E-15	4.05E-16	320	6.82E-15	4.12E-15	1.17E-15

Table S19: Bimolecular rate constant  $k_b$  in ( $\text{cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$ ) for  $(\text{H}_2\text{O})_2$  catalyzed channels for THAT-WD path for  $\text{CH}_2\text{OO} + \text{cis/trans-HONO}$  within temperature range 213-320K.

cis-HONO				trans-HONO			
Temp (K)	Path A	Path B	Path C	Temp (K)	Path A	Path B	Path C
213	2.74E-07	4.30E-08	7.01E-10	213	4.66E-07	1.95E-07	4.44E-09
216	1.90E-07	3.20E-08	5.67E-10	216	3.27E-07	1.39E-07	3.49E-09
219	1.34E-07	2.39E-08	4.62E-10	219	2.31E-07	9.95E-08	2.77E-09
224	7.55E-08	1.51E-08	3.32E-10	224	1.33E-07	5.83E-08	1.90E-09
235	2.34E-08	5.84E-09	1.69E-10	235	4.24E-08	1.95E-08	8.88E-10
250	5.61E-09	1.84E-09	7.46E-11	250	1.06E-08	5.15E-09	3.52E-10
259	2.57E-09	9.83E-10	4.79E-11	259	4.96E-09	2.49E-09	2.13E-10
265	1.58E-09	6.62E-10	3.63E-11	265	3.08E-09	1.58E-09	1.56E-10
278	5.87E-10	2.99E-10	2.08E-11	278	1.18E-09	6.32E-10	8.29E-11
280	5.08E-10	2.67E-10	1.92E-11	280	1.03E-09	5.53E-10	7.56E-11
290	2.55E-10	1.53E-10	1.30E-11	290	5.25E-10	2.92E-10	4.88E-11
298	1.52E-10	1.01E-10	9.76E-12	298	3.17E-10	1.81E-10	3.51E-11
300	1.34E-10	9.16E-11	9.11E-12	300	2.81E-10	1.61E-10	3.25E-11
310	7.32E-11	5.66E-11	6.52E-12	310	1.57E-10	9.22E-11	2.22E-11
320	4.17E-11	3.61E-11	4.77E-12	320	9.06E-11	5.47E-11	1.56E-11

Table S20: Concentration of  $\text{H}_2\text{O}$  and  $(\text{H}_2\text{O})_2$  at 20% RH and 100% RH with in temperature range of 280-320 K

Temp (K)	$[\text{H}_2\text{O}]$		$[(\text{H}_2\text{O})_2]$	
	20% RH	100% RH	20% RH	100% RH
280	$5.16 \times 10^{+16}$	$2.58 \times 10^{+17}$	$8.18 \times 10^{+12}$	$2.04 \times 10^{+14}$
290	$9.56 \times 10^{+16}$	$4.78 \times 10^{+17}$	$2.36 \times 10^{+13}$	$5.91 \times 10^{+14}$
298	$1.55 \times 10^{+17}$	$7.73 \times 10^{+17}$	$5.44 \times 10^{+13}$	$1.36 \times 10^{+15}$
300	$1.72 \times 10^{+17}$	$8.58 \times 10^{+17}$	$6.50 \times 10^{+13}$	$1.62 \times 10^{+15}$
310	$2.92 \times 10^{+17}$	$1.46 \times 10^{+18}$	$1.63 \times 10^{+14}$	$4.06 \times 10^{+15}$
320	$4.70 \times 10^{+17}$	$2.35 \times 10^{+18}$	$3.71 \times 10^{+14}$	$9.24 \times 10^{+15}$

Table S21: Bimolecular rate constant  $k_{bi}$  (in  $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ) for uncatalyzed reaction of  $\text{CH}_2\text{OO} + \text{H}_2\text{O}$  within the temperature range 213–320 K.

Temp (K)	$K_{eq}$	$k_{uni}$	$k_b$
213	4.38E-19	6.85E+02	3.00E-16
216	3.47E-19	9.01E+02	3.13E-16
219	2.77E-19	1.18E+03	3.26E-16
224	1.93E-19	1.81E+03	3.48E-16
235	9.20E-20	4.34E+03	3.99E-16
250	3.74E-20	1.27E+04	4.73E-16
259	2.30E-20	2.26E+04	5.20E-16
265	1.69E-20	3.26E+04	5.51E-16
278	9.17E-21	6.79E+04	6.22E-16
280	8.39E-21	7.55E+04	6.33E-16
290	5.48E-21	1.26E+05	6.90E-16
298	3.99E-21	1.85E+05	7.36E-16
300	3.69E-21	2.03E+05	7.48E-16
310	2.56E-21	3.16E+05	8.08E-16
320	1.82E-21	4.78E+05	8.69E-16

Table S22: Termolecular rate constant  $k_t$  in ( $\text{cm}^6 \text{ molecule}^{-2} \text{ sec}^{-1}$ ) for reaction  $\text{CH}_2\text{OO} + \text{H}_2\text{O}$  catalyzed by HONO within temperature range 213-320K.

Temp (K)	PATH A				PATH B				PATH C			
	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt	keq1	keq2	kuni	kt
213	1.66E-18	3.31E-18	3.17E+09	1.74E-26	7.88E-20	6.97E-17	3.17E+09	1.74E-26	4.38E-19	1.26E-17	3.17E+09	1.74E-26
216	1.28E-18	2.54E-18	3.37E+09	1.09E-26	6.48E-20	5.01E-17	3.37E+09	1.09E-26	3.47E-19	9.35E-18	3.37E+09	1.09E-26
219	9.88E-19	1.97E-18	3.57E+09	6.94E-27	5.36E-20	3.63E-17	3.57E+09	6.95E-27	2.77E-19	7.02E-18	3.57E+09	6.94E-27
224	6.55E-19	1.31E-18	3.92E+09	3.35E-27	3.95E-20	2.17E-17	3.92E+09	3.35E-27	1.93E-19	4.44E-18	3.92E+09	3.35E-27
235	2.83E-19	5.64E-19	4.74E+09	7.56E-28	2.12E-20	7.53E-18	4.74E+09	7.56E-28	9.20E-20	1.74E-18	4.74E+09	7.57E-28
250	1.03E-19	2.03E-19	5.95E+09	1.24E-28	9.99E-21	2.08E-18	5.95E+09	1.24E-28	3.74E-20	5.56E-19	5.95E+09	1.24E-28
259	5.92E-20	1.17E-19	6.72E+09	4.64E-29	6.65E-21	1.04E-18	6.72E+09	4.64E-29	2.30E-20	3.00E-19	6.72E+09	4.64E-29
265	4.20E-20	8.25E-20	7.26E+09	2.51E-29	5.15E-21	6.72E-19	7.26E+09	2.51E-29	1.69E-20	2.04E-19	7.26E+09	2.51E-29
278	2.10E-20	4.10E-20	8.45E+09	7.29E-30	3.09E-21	2.79E-19	8.45E+09	7.29E-30	9.17E-21	9.41E-20	8.45E+09	7.29E-30
280	1.90E-20	3.71E-20	8.64E+09	6.09E-30	2.87E-21	2.46E-19	8.64E+09	6.10E-30	8.39E-21	8.41E-20	8.64E+09	6.09E-30
290	1.18E-20	2.28E-20	9.60E+09	2.59E-30	2.02E-21	1.34E-19	9.60E+09	2.58E-30	5.48E-21	4.91E-20	9.60E+09	2.59E-30
298	8.25E-21	1.59E-20	1.04E+10	1.36E-30	1.55E-21	8.46E-20	1.04E+10	1.36E-30	3.99E-21	3.29E-20	1.04E+10	1.36E-30
300	7.57E-21	1.46E-20	1.06E+10	1.17E-30	1.45E-21	7.58E-20	1.06E+10	1.17E-30	3.69E-21	2.98E-20	1.06E+10	1.17E-30
310	5.01E-21	9.58E-21	1.16E+10	5.55E-31	1.07E-21	4.47E-20	1.16E+10	5.55E-31	2.56E-21	1.88E-20	1.16E+10	5.55E-31
320	3.41E-21	6.48E-21	1.26E+10	2.78E-31	8.09E-22	2.73E-20	1.26E+10	2.78E-31	1.82E-21	1.22E-20	1.26E+10	2.78E-31

Table S23: Bimolecular rate constant  $k_b$  in ( $\text{cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$ ) for reaction  $\text{CH}_2\text{OO} + \text{H}_2\text{O}$  catalyzed by HONO within temperature range 213-320K.

Temp (K)	Path A	Path B	Path C
213	1.05E-08	2.21E-07	3.99E-08
216	8.57E-09	1.69E-07	3.15E-08
219	7.03E-09	1.30E-07	2.51E-08
224	5.12E-09	8.49E-08	1.74E-08
235	2.67E-09	3.56E-08	8.22E-09
250	1.21E-09	1.24E-08	3.31E-09
259	7.84E-10	6.98E-09	2.02E-09
265	5.98E-10	4.87E-09	1.48E-09
278	3.47E-10	2.36E-09	7.95E-10
280	3.20E-10	2.12E-09	7.26E-10
290	2.19E-10	1.28E-09	4.72E-10
298	1.65E-10	8.78E-10	3.41E-10
300	1.54E-10	8.01E-10	3.16E-10
310	1.11E-10	5.17E-10	2.17E-10
320	8.14E-11	3.43E-10	1.53E-10

Table S24: Bimolecular rate constant  $k_b$  in ( $\text{cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$ ) for  $\text{CH}_2\text{OO} + \text{H}_2\text{O}$  uncatalyzed reaction and  $k_{eff}$  for HONO catalyzed reaction in temperature range 280-320K.

Temp (K)	$k_b^{uncat}$	$k_{eff}$
280	6.33E-16	6.09E-20
290	6.90E-16	2.59E-20
298	7.36E-16	1.36E-20
300	7.48E-16	1.17E-20
310	8.08E-16	5.55E-21
320	8.69E-16	2.78E-21

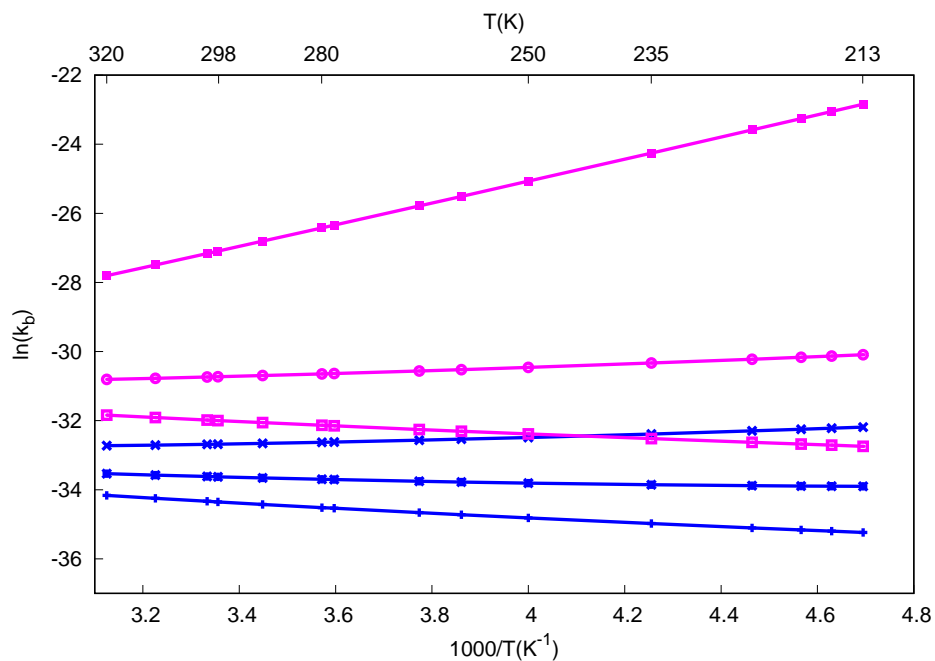


Figure S1: Arrhenius plot for SHAT-WM channel of the bimolecular rate constants ( $k_b$ ) for the  $\text{CH}_2\text{OO} + \text{cis/trans-HONO}$  reaction in presence of  $\text{H}_2\text{O}$  within the temperature range of 213 K to 320 K for the A(P1), path B(P2) and path C(P3).

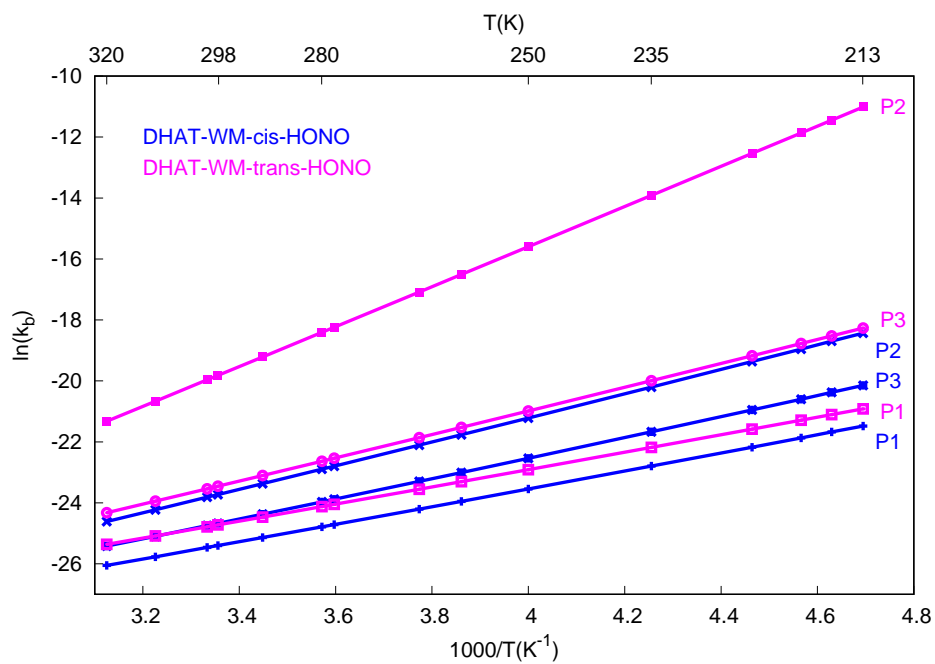


Figure S2: Arrhenius plot for DHAT-WM channel of the bimolecular rate constants ( $k_b$ ) for the  $\text{CH}_2\text{OO} + \text{cis/trans-HONO}$  reaction in presence of  $\text{H}_2\text{O}$  within the temperature range of 213 K to 320 K for the A(P1), path B(P2) and path C(P3).



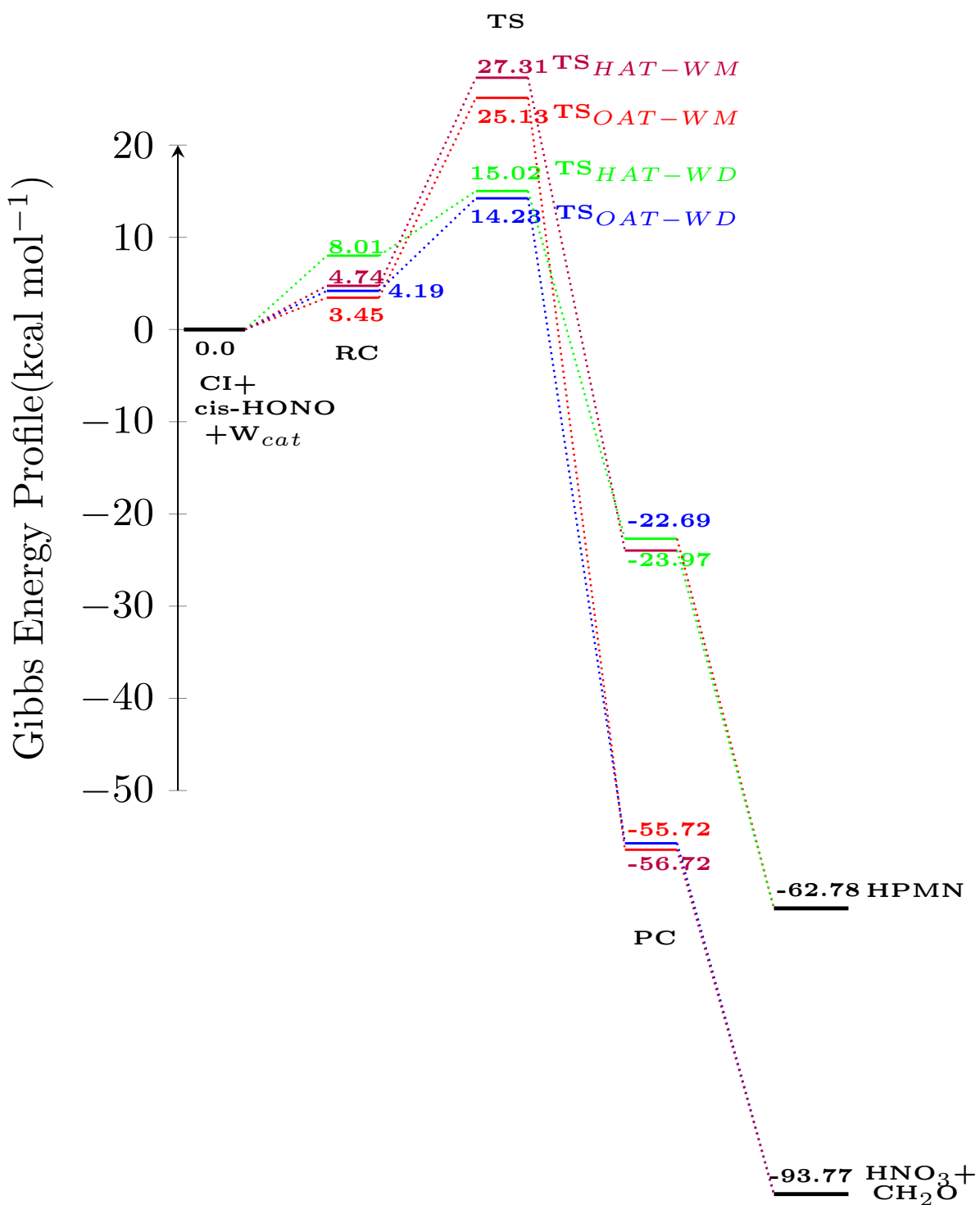


Figure S3: Gibbs free energy profile for CH<sub>2</sub>OO + cis-HONO reaction in presence of H<sub>2</sub>O and (H<sub>2</sub>O)<sub>2</sub> calculated at CCSD(T)/CBS//M06-2X/aug-cc-pVTZ level of theory.

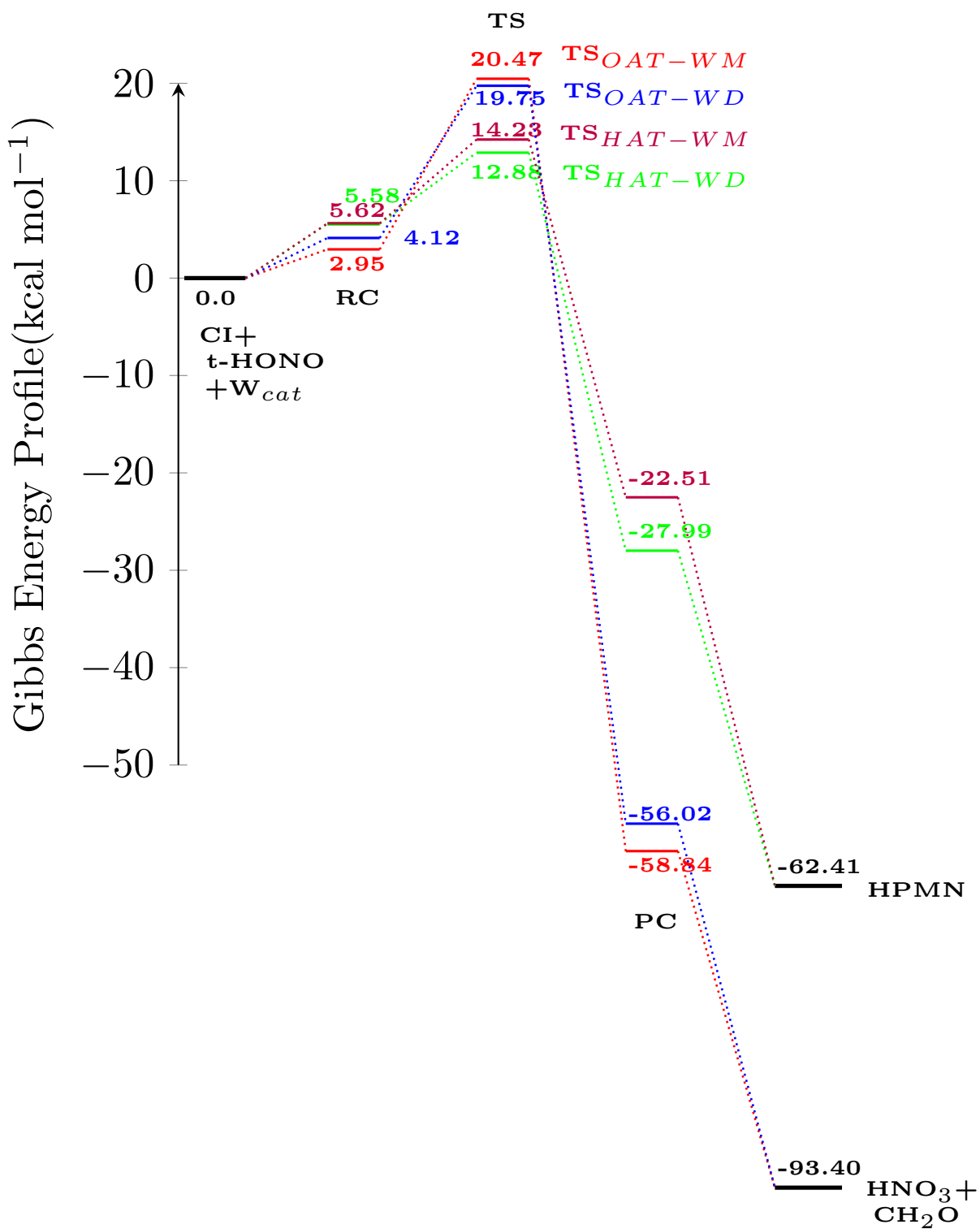


Figure S4: Gibbs free energy profile for  $\text{CH}_2\text{OO} + \text{trans-HONO}$  reaction in presence of  $\text{H}_2\text{O}$  and  $(\text{H}_2\text{O})_2$  calculated at CCSD(T)/CBS//M06-2X/aug-cc-pVTZ level of theory.

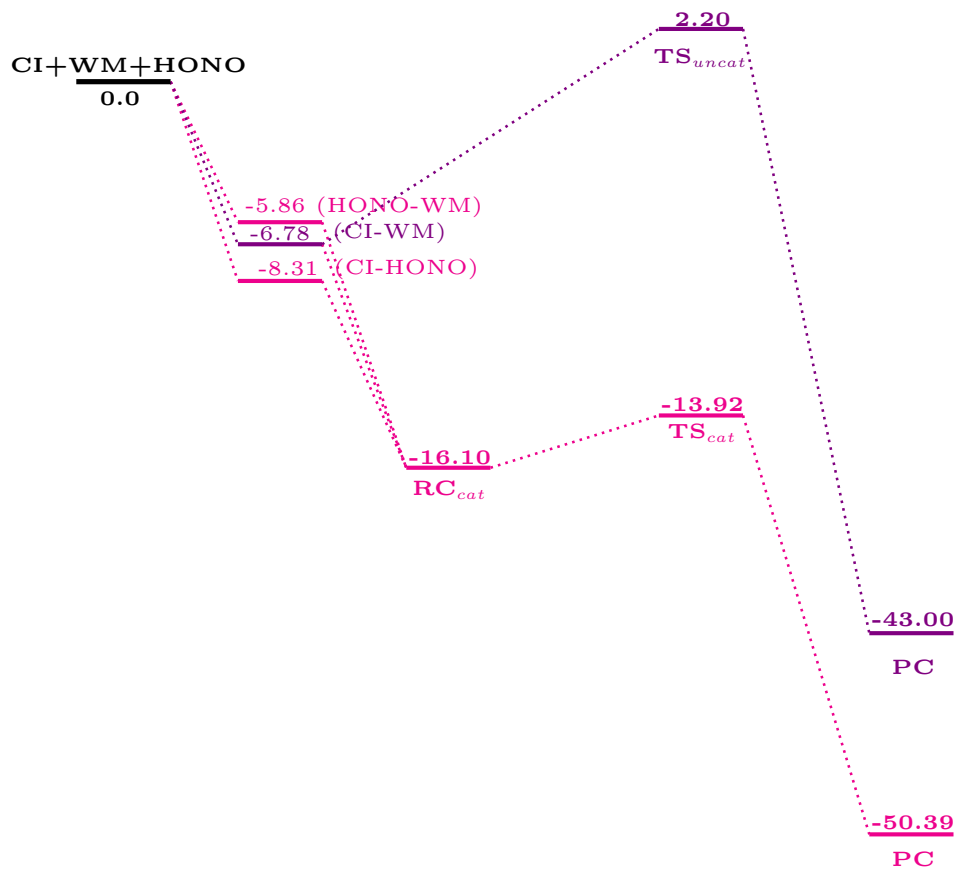


Figure S5: Potential free energy surface for  $\text{CH}_2\text{OO} + \text{H}_2\text{O}$  uncatalysed and HONO-catalyzed reaction calculated at CCSD(T)/CBS//M06-2X/aug-cc-pVTZ level of theory.