Supporting Information

Interfacial Ozone Chemistry Enables Aromatic Oxidation in Microdroplets

Lian Xue[+],Boyu Zhu[+], Peng Zheng, Xinyao Li, Kaiyu Geng,* Jiao Geng,* Xingbang Hu,*

[1] State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, PR China

[*]Corresponding author E-mail: kaiyugeng@nju.edu.cn; gengjiao@nju.edu.cn; huxb@nju.edu.cn

[+]Lian Xue and Boyu Zhu share the first authorship.

List of Contents

32. **Table S3.** A series of microdroplet reactions of naphthalene oxidation carried out under different conditions.
33. **References**

1. Chemicals

Naphthalene (NA) and methanol (CH_3OH, AR) were obtained from Nanjing Juyou Scientific Equipment Co., Ltd., dimethyl phthalate (DP), phosphpric acid (H_3PO_4) and ethyl acetate (EA) were purchased from Nanjing Shoude Biotechnology Co., Ltd., 5-dimethyl-1-pyrroline N-oxide (97%, DMPO) was purchased from Meili (Shanghai) Chemical Technology Co., Ltd., and indigo disulfonate sodium (IDS) was purchased from Nanjing Wanqing Glass Instrument Co., Ltd. Disodium hydrogen phosphate (Na_2HPO_4), Tert-butanol (TBA), 2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO) and Sodium Iodide (NaI) were purchased from Shanghai Bide Pharmaceutical Technology Co., Ltd. Deionized water is provided by Milli-Q from Nanjing University. All chemicals are used as is without further purification.

2. General procedures

Droplets are generated by atomizers (ultrasonic power). Firstly, dissolve naphthalene in a 1:5.5 methanol water mixed solution to form a homogeneous solution. Then, inject the solution into the reactor equipped with an atomizer, ensuring that the atomizer is completely submerged in the solution. At room temperature and in an air atmosphere, droplets are sprayed from bottom to top and then fall back to the surface of the solution under the action of gravity, forming a cycle. This process lasts for 4 hours to prepare dimethyl phthalate.

To comprehensively explore the factors influencing the reaction, a series of microdroplet experiments were conducted under different conditions. To assess the roles of O_2 and H_2O_2, reactions were performed using N_2, O_2, and H_2O_2 as comparative systems, with the N_2 + H_2O_2 setup specifically designed to eliminate the possible interference of O_3, which could form O_2 via microdroplet reactions in an air atmosphere. To further exclude the contribution of H_2O_2, a control experiment with catalase was performed to specifically decompose H_2O_2. To distinguish ozone-driven chemistry from general reactive oxygen species (ROS)-mediated oxidation, radical quenching experiments were performed using tert-butanol (TBA, a selective hydroxyl radical scavenger) and 2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO, a broad-spectrum radical scavenger). To compare the E-factor and energy input with the catalytic aerobic oxidation method, we conducted oxidation experiments using an ozone generator.

Additionally, the impact of temperature was examined by varying it across 30 ℃, 40 ℃, 50 ℃, and 60 ℃. The effect of atomization power was evaluated by adjusting it to 10W, 20W, and 30W. Furthermore, to determine the influence of ultrasound, three different conditions were compared: ultrasound + non-spray, non-ultrasound + spray, and ultrasound + spray. To enhance the reliability of the results, all experiments were conducted in triplicate.

3. Measure the size of microdroplets

We used a high-speed camera equipped with a high-magnification lens (Phato, USA) to capture the microdroplets (Fig. 1a). Since the high-speed camera could not clearly capture the microdroplets in a single frame, we attempted to observe and measure them using a microscope. Specifically, the microdroplets floating in the air were encapsulated in an immiscible oil phase, and the system was then observed under the microscope (Fig. 1b).

4. Product detection

Product analysis was performed using a Shimadzu GC-MS-QP2202NX. The concentration of DP was determined using a Shimadzu GC-2014C gas chromatograph. NMR spectra were recorded using a Bruker DPX 400 MHz spectrometer with DMSO-d6 as the solvent. The structures of NA and DP were determined by ^{1}H and ^{13}C NMR. Isopropanol was used as the internal standard, and the yield of DP was calculated based on ^{1}H NMR (Fig. S7).

5. O_3 Detection Method

Ozone (O_3) reacts rapidly with indigo disulfonate sodium (IDS), causing decolorization under acidic conditions. The absorbance change at 610 nm is linearly correlated with O_3 concentration, making it suitable for rapid detection. In contrast, hydrogen peroxide (H_2O_2) can also induce IDS decolorization, but at a much slower rate. If measurements are conducted within 6h of reagent addition, H_2O_2 interference can be neglected.[1]
When applied to the microdroplet system under an O_2 atmosphere, ultraviolet-visible spectroscopy (UV-Vis) show that the characteristic absorption peak of IDS at 610 nm decreases rapidly with reaction time,[1-2] with noticeable decolorization occurring within about 1.25 hours, turning the solution from deep blue to almost colorless (**Fig. 4a**).[3] In contrast, under the same concentration of H_2O_2, even when the reaction time is extended to 10 hours, the change in absorption intensity is minimal, with almost no noticeable decolorization. Although hydrogen peroxide (H_2O_2) can also induce the decolorization of IDS under specific conditions, its reaction rate is much slower than that of O_3. Previous literature reports that during the first 6 hours after reagent addition, the influence of H_2O_2 is negligible,[1] ensuring that the observed decolorization phenomenon is primarily attributed to the oxidation by O_3.

To further verify the presence of ozone, sodium iodide (NaI) was used as an additional probe. The strong oxidant generated in microdroplets oxidized I^- to IO_3^- (m/z = 174.88), indicating the formation of a highly active interfacial oxidant capable of multielectron oxidation, which is consistent with typical ozone-mediated chemistry.[2] This method is well-supported by recent studies demonstrating that NaI can be selectively oxidized to IO_x^- species by ozone generated in charged water microdroplets.[4]

In this experiment, IDS was first added in a phosphoric acid-disodium hydrogen phosphate (H_3PO_4-Na_2HPO_4) solution. The prepared solution was then introduced into the reaction chamber and subjected to ultrasonic nebulization for approximately 1h in a recirculating spray system. Subsequently, UV-Vis spectroscopy (Shimadzu UV-2600i) and electrospray ionization mass spectrometry (ESI-MS, Thermo Fisher) were performed, with all analyses completed within 2h. UV-Vis spectroscopy showed a significant decrease in absorbance at 610 nm, accompanied by a color change from blue to colorless, confirming the in-situ generation of O_3 in microdroplets. Additionally, ESI-MS detected a oxidation product of IDS by O_3 at m/z = 226.0 (Fig. 4c), further providing evidence of O_3 presence.

Notably, we also directly captured the primary ozonide (POZ) intermediate of naphthalene ozonolysis by high-resolution mass spectrometry. The observation of this short-lived intermediate provides direct mechanistic evidence for the reaction between naphthalene and in-situ generated ozone, consistent with the well-established ozonolysis pathway in microdroplet systems.[5]

6. Radical Detection

The methyl radical ($\bullet CH_3$) was trapped by DMPO and detected using a Bruker A300 electron spin resonance (EPR) spectrometer and Thermo Fisher electrospray ionization mass spectrometry (ESI-MS).

7. Calculation methods

The Density Function Theory (DFT) calculations were conducted using the Gaussian16 and Gaussian09 software package employing the B3LYP hybrid functional for electron exchange and correlation with Empirical Dispersion = GD3BJ keyword, and utilizing the 6-311+G(d, p) basis set for all atoms [abbr: B3LYP/6-311+G(d, p)]. The impact of an oriented external electric field (OEEF) was initially investigated in Gaussian 16, defining the EEF axis, direction, and magnitude with the "Field = M ± N" keyword. Energy calculations and Zero-point energy (ZPE) correction have been done by using the same level of theory.[2, 4]

Fig. S1 (a) Liquid mixtures used for microdroplets reaction and (b) Ultrasonic atomization device for synthesizing dimethyl phthalate microdroplets.

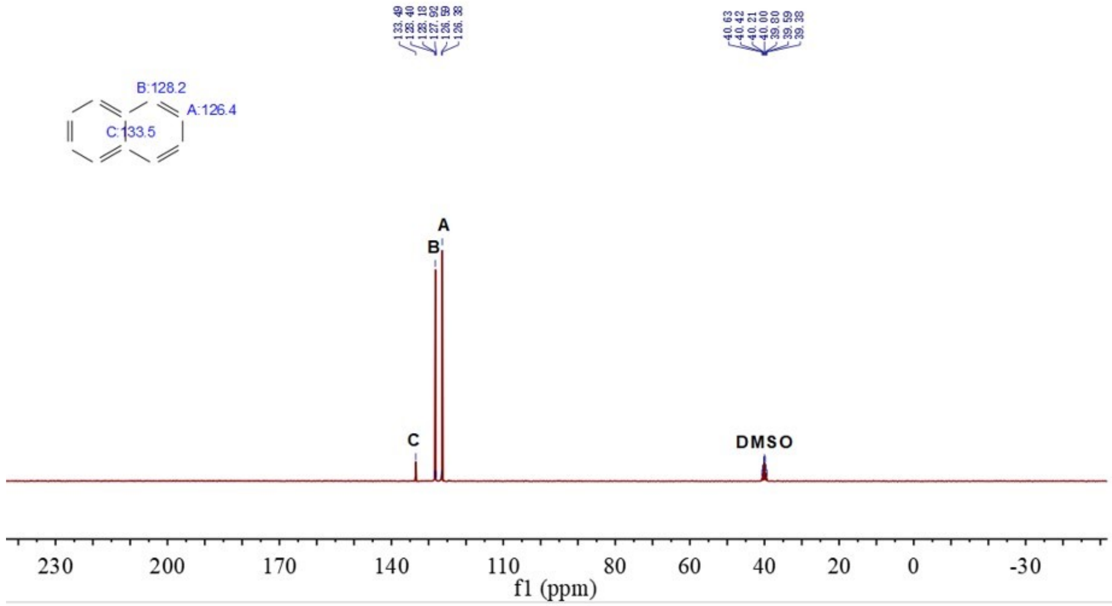


Fig. S2 ^{13}C NMR spectrum of naphthalene.

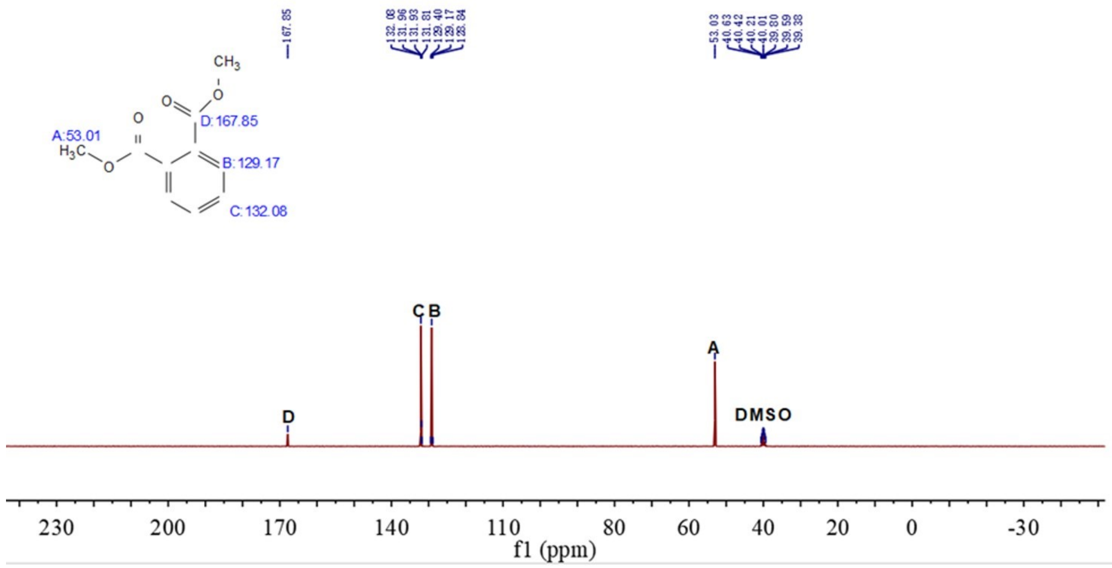


Fig. S3 ^{13}C NMR spectrum of dimethyl phthalate.

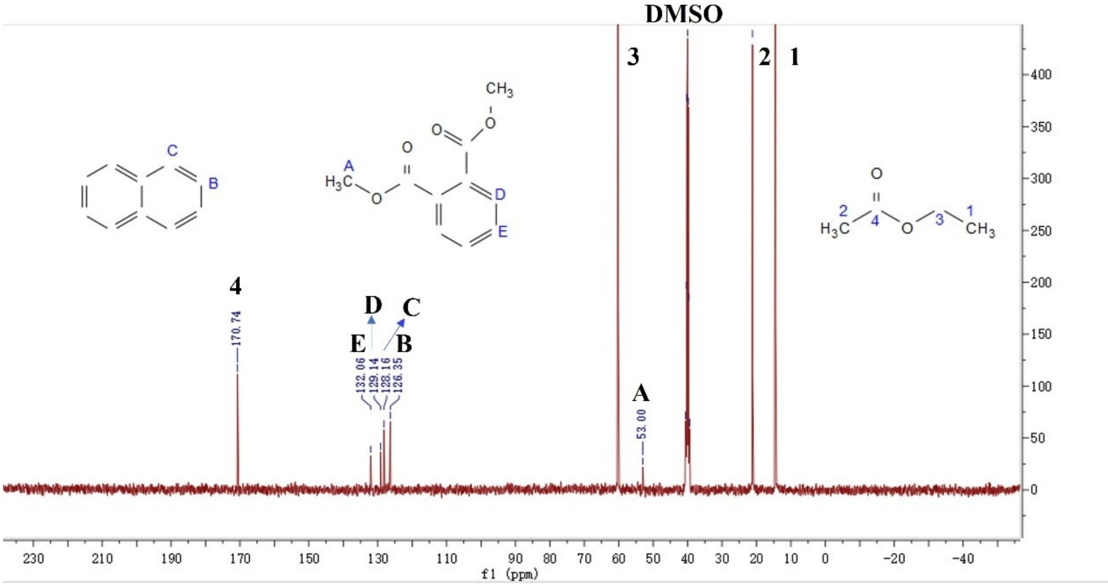


Fig. S4 ^{13}C NMR spectra of naphthalene oxidation to dimethyl phthalate in cyclic microdroplets reaction.

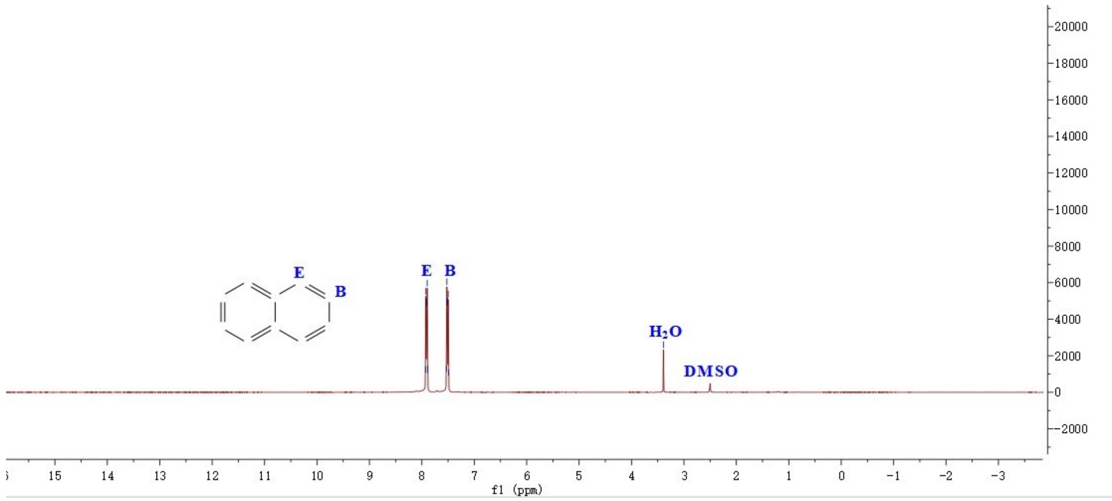


Fig. S5 ^{1}H NMR spectrum of naphthalene.

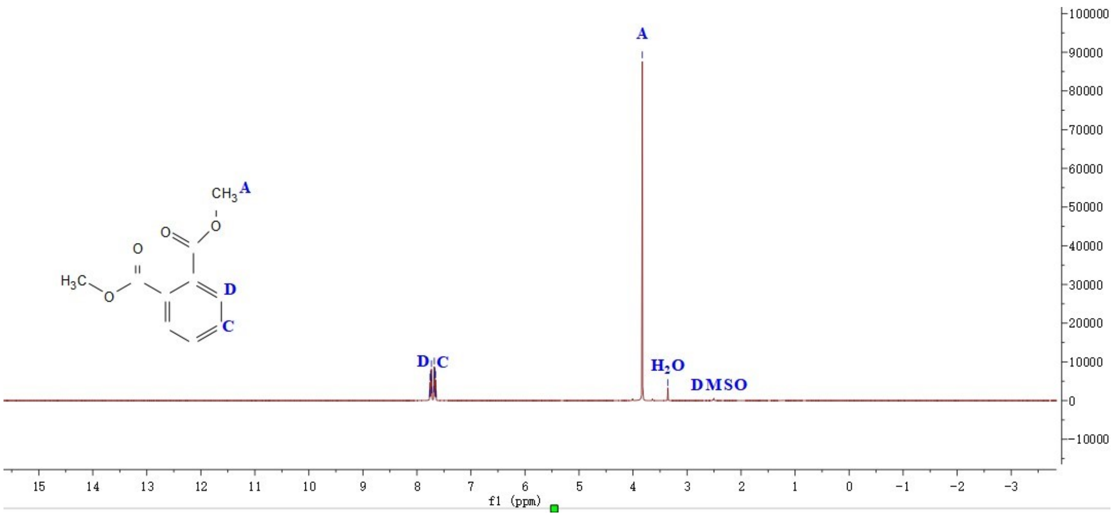


Fig. S6 ^{1}H NMR spectrum of dimethyl phthalate.

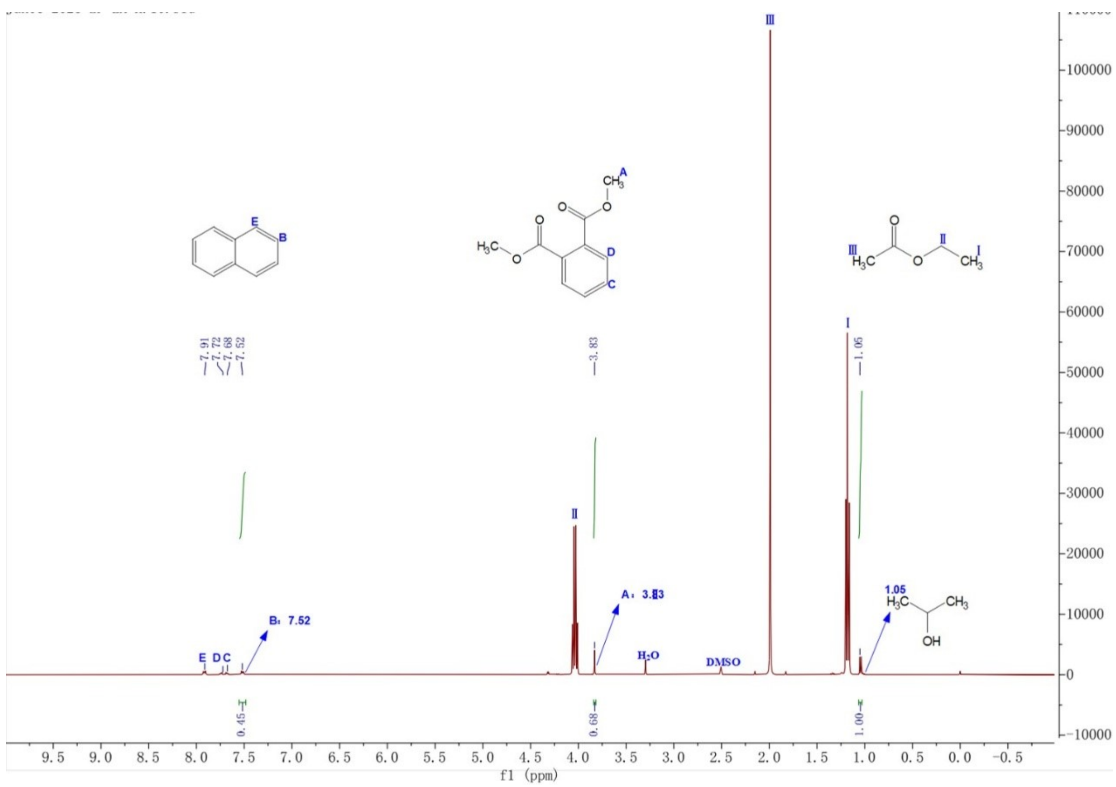


Fig. S7 ^{1}H NMR spectra of naphthalene oxidation to dimethyl phthalate in cyclic microdroplets reaction.

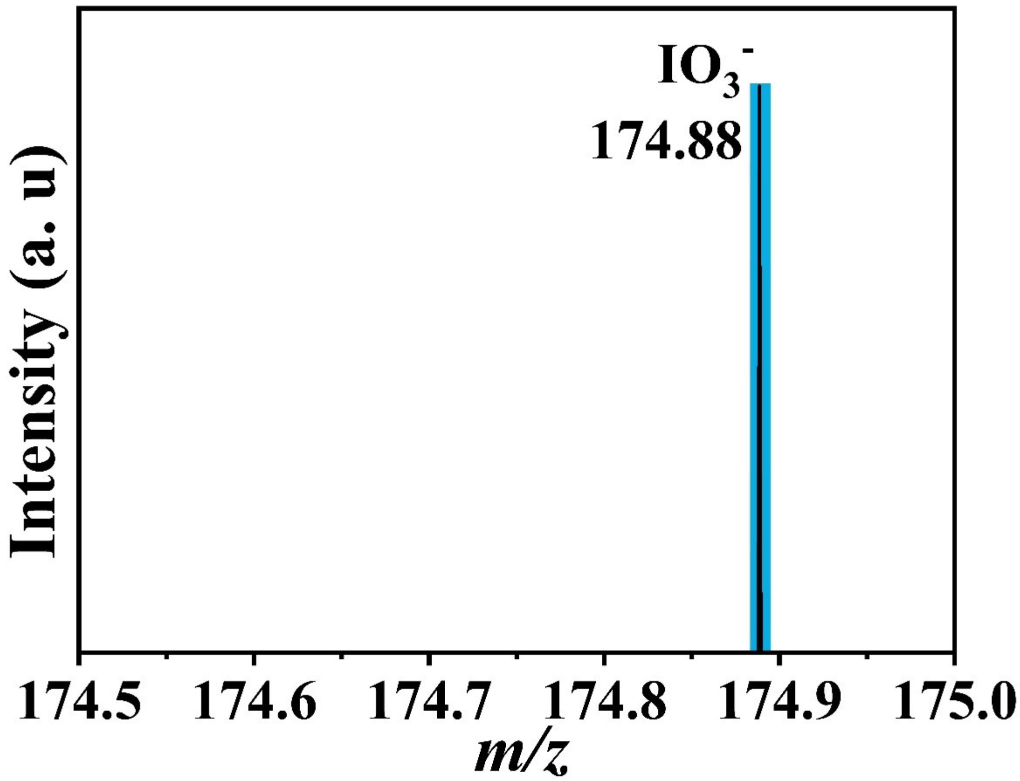


Fig. S8 High resolution mass spectrometry image of microdroplet reaction after spraying NaI/H_2O solution.

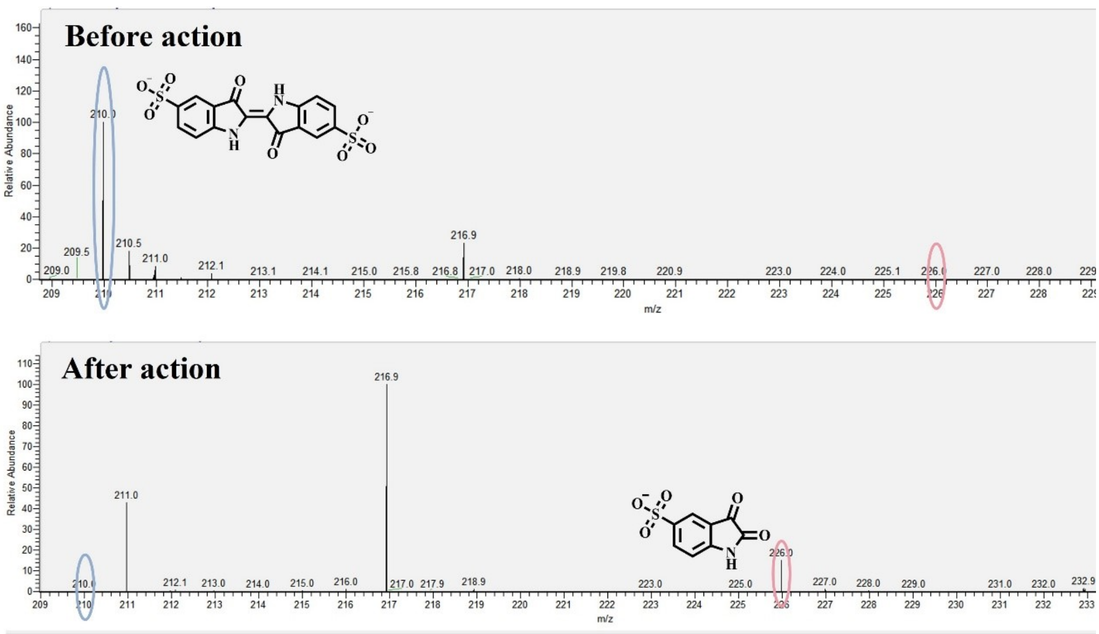


Fig. S9 High resolution mass spectrometry of IDS before and after oxidation reaction in microdroplets.

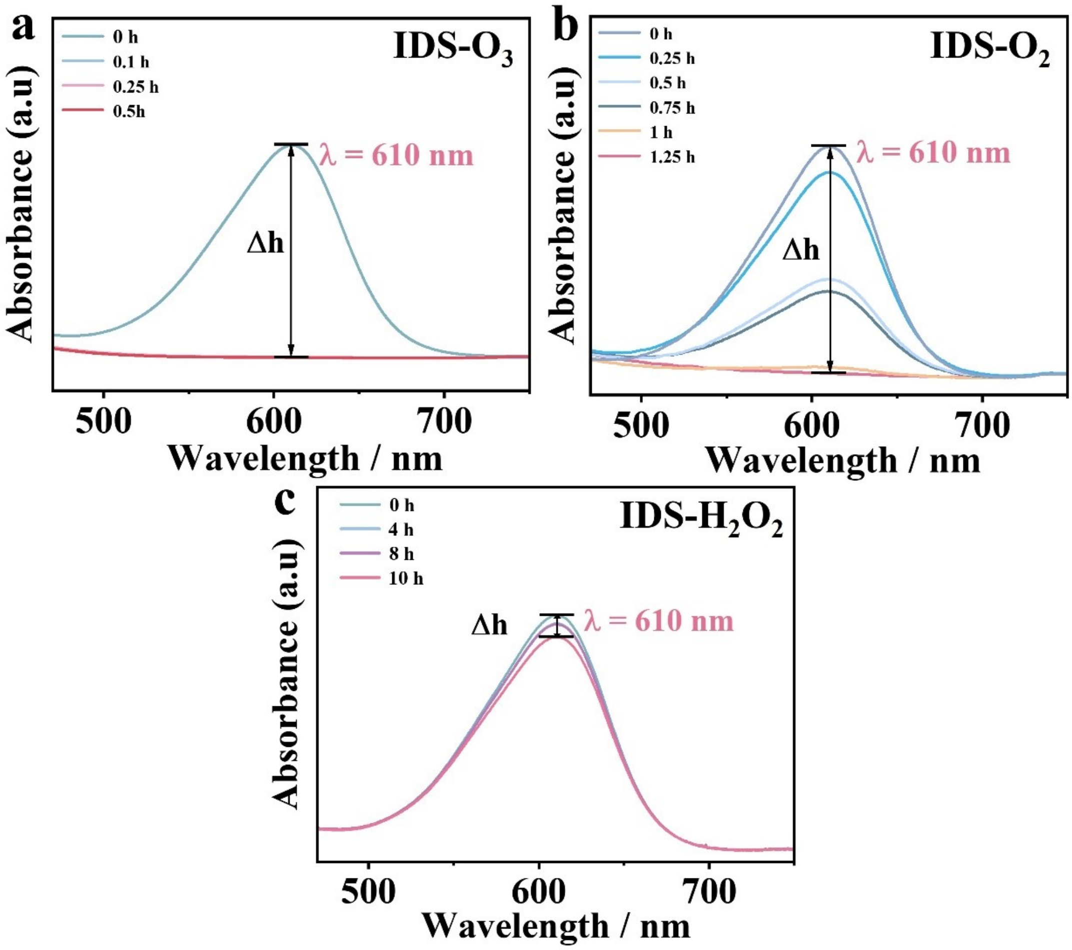


Fig. S10 UV visible absorption spectra of (a) IDS-O_3, (b) IDS-O_2 and (c) IDS-H_2O_2 at different reaction times. Δh represents the absorbance change at 610 nm, defined as Δh=A_t-$A_{0,}$ t (t =0.1, 0.25 h, 0.5 h, 0.75 h, 1 h, 1.25 h, 4 h, 8 h, 10 h), A_0 is the absorbance at 0 h.

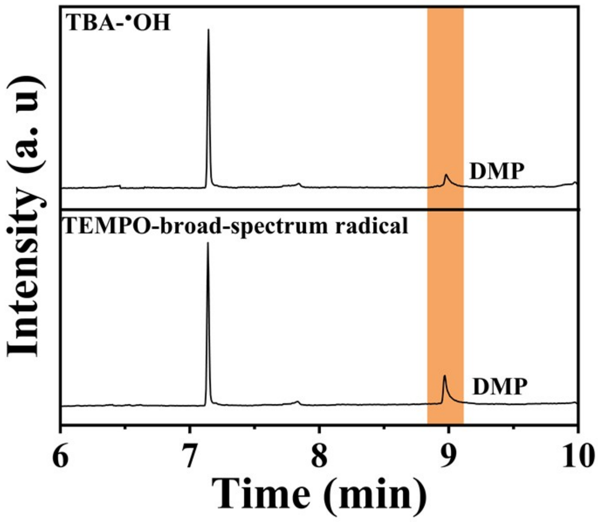


Fig. S11 Radical quenching experiments using tert-butanol (TBA) and TEMPO.

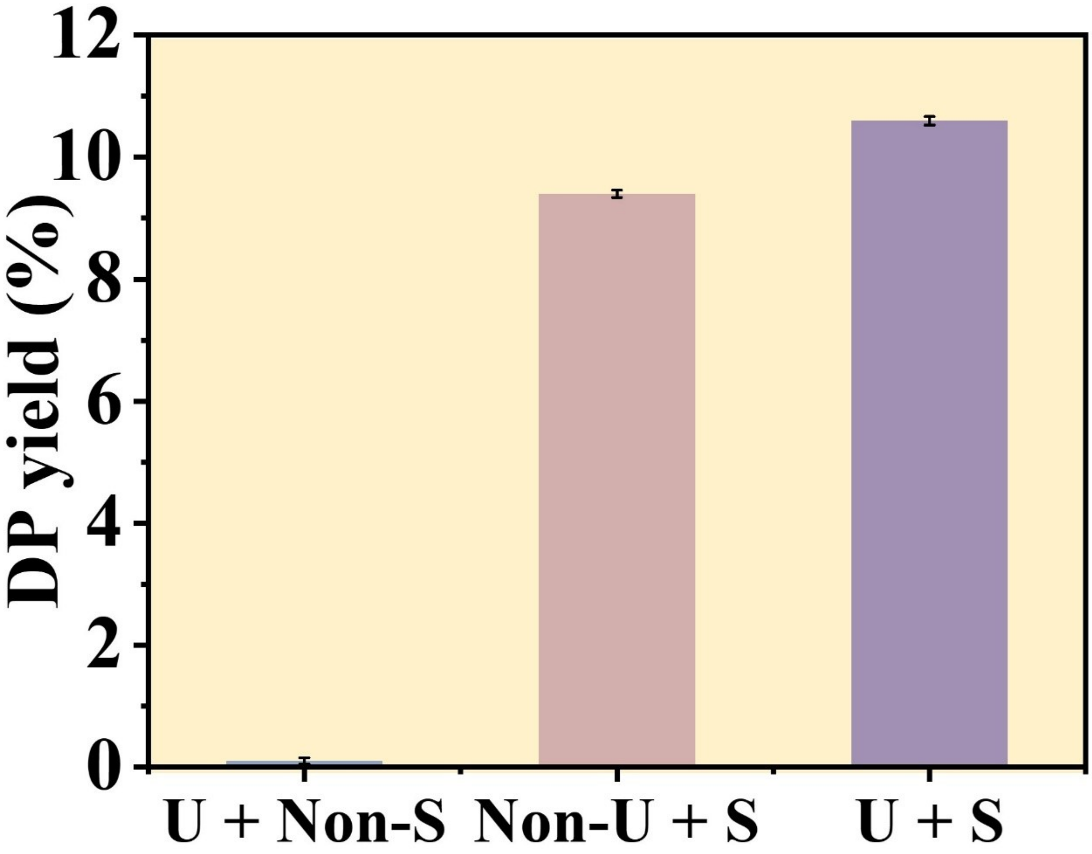


Fig. S12 Ultrasonic + non spray, non ultrasonic + spray and ultrasonic + spray were used for the microdroplets reaction of naphthalene oxidation to dimethyl phthalate in air atmosphere.

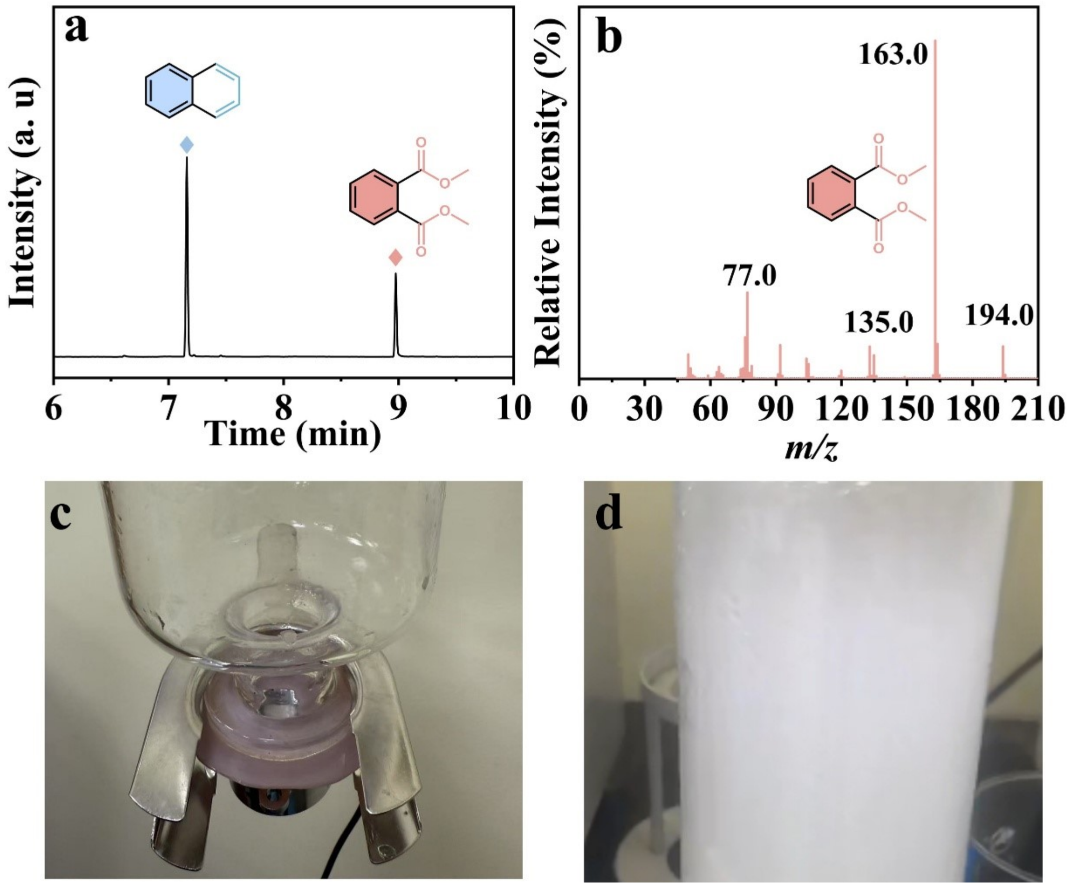


Fig. S13 (a) Gas chromatogram and (b) mass spectrum of spontaneous oxidation of naphthalene droplets produced in an inverted spray device (c) and (d).

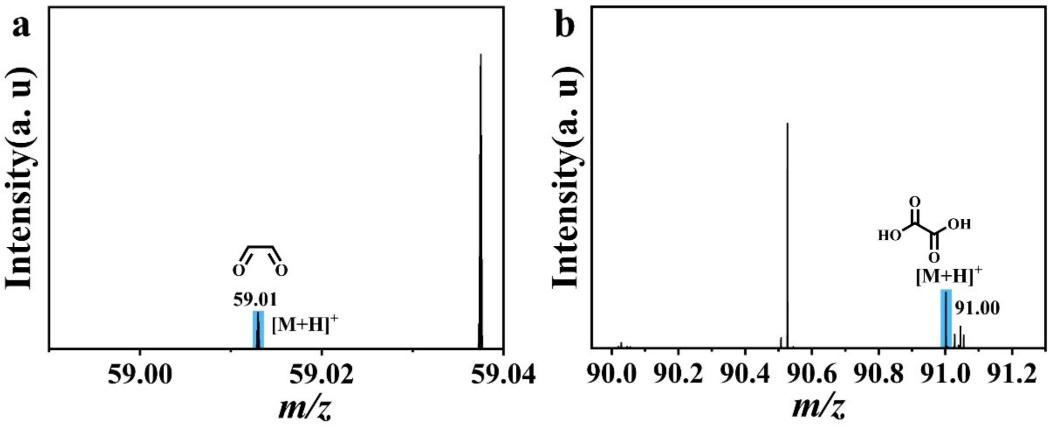


Fig. S14 High resolution mass spectrometry of glyoxal and oxalic acid.

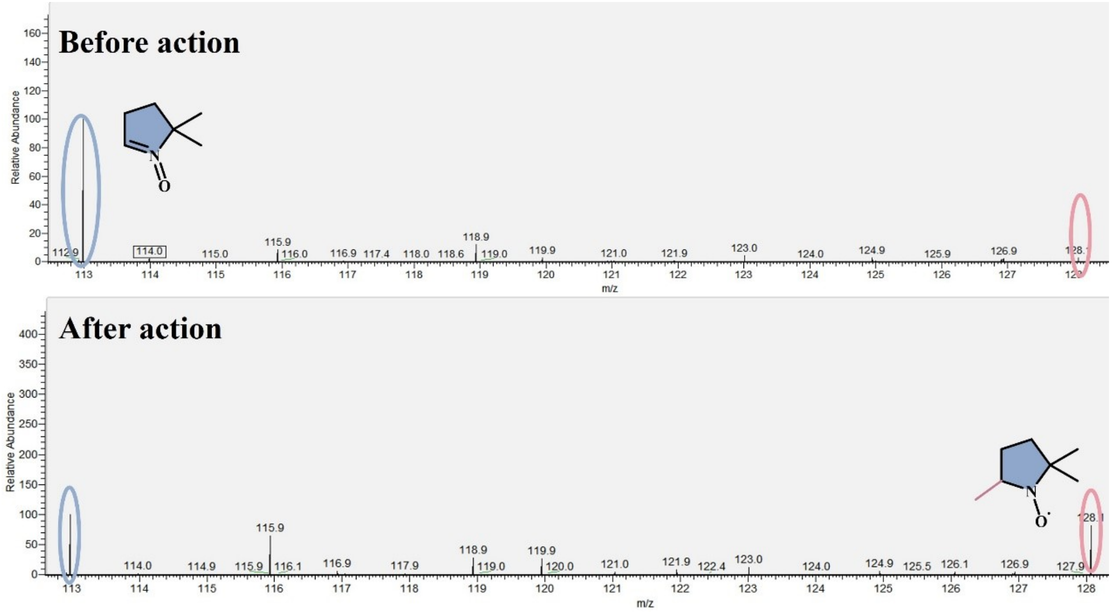


Fig. S15 High resolution mass spectrometry of DMPO capturing $\cdot CH_3$ before and after microdroplet reaction.

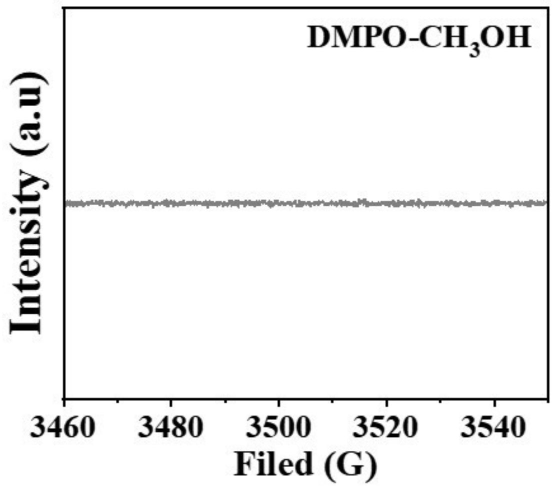


Fig. S16 EPR spectrum of pure CH_3OH-DMPO.

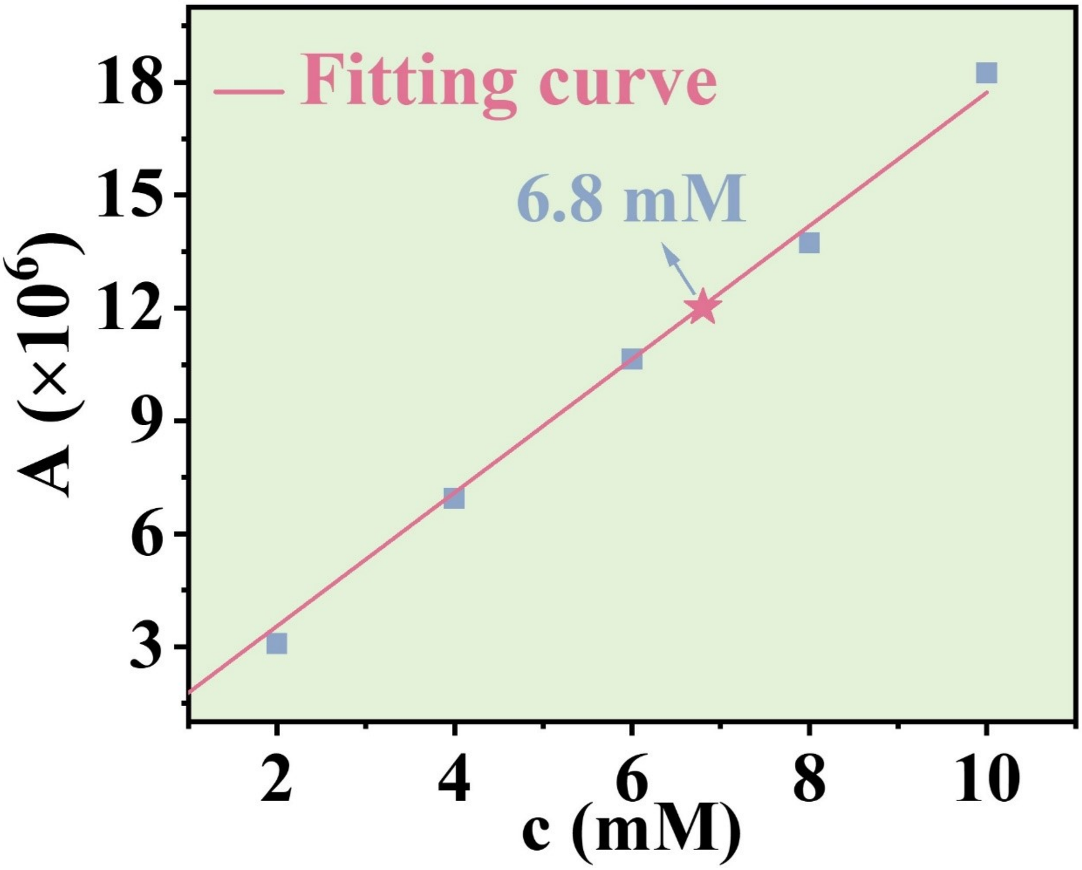


Fig. S17 The calibration curves of dimethyl phthalate with 5 concentrations (2 mM, 4 mM, 6 mM, 8 mM, and 10 mM) using a gas chromatography.

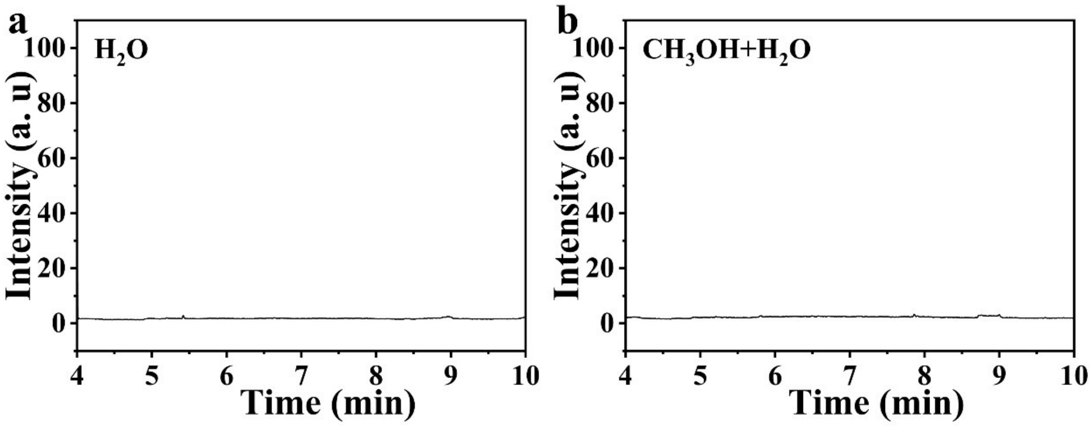


Fig. S18 (a) GC-MS chromatogram of microdroplet control experiment of pure water and (b) water-methanol mixed solution.

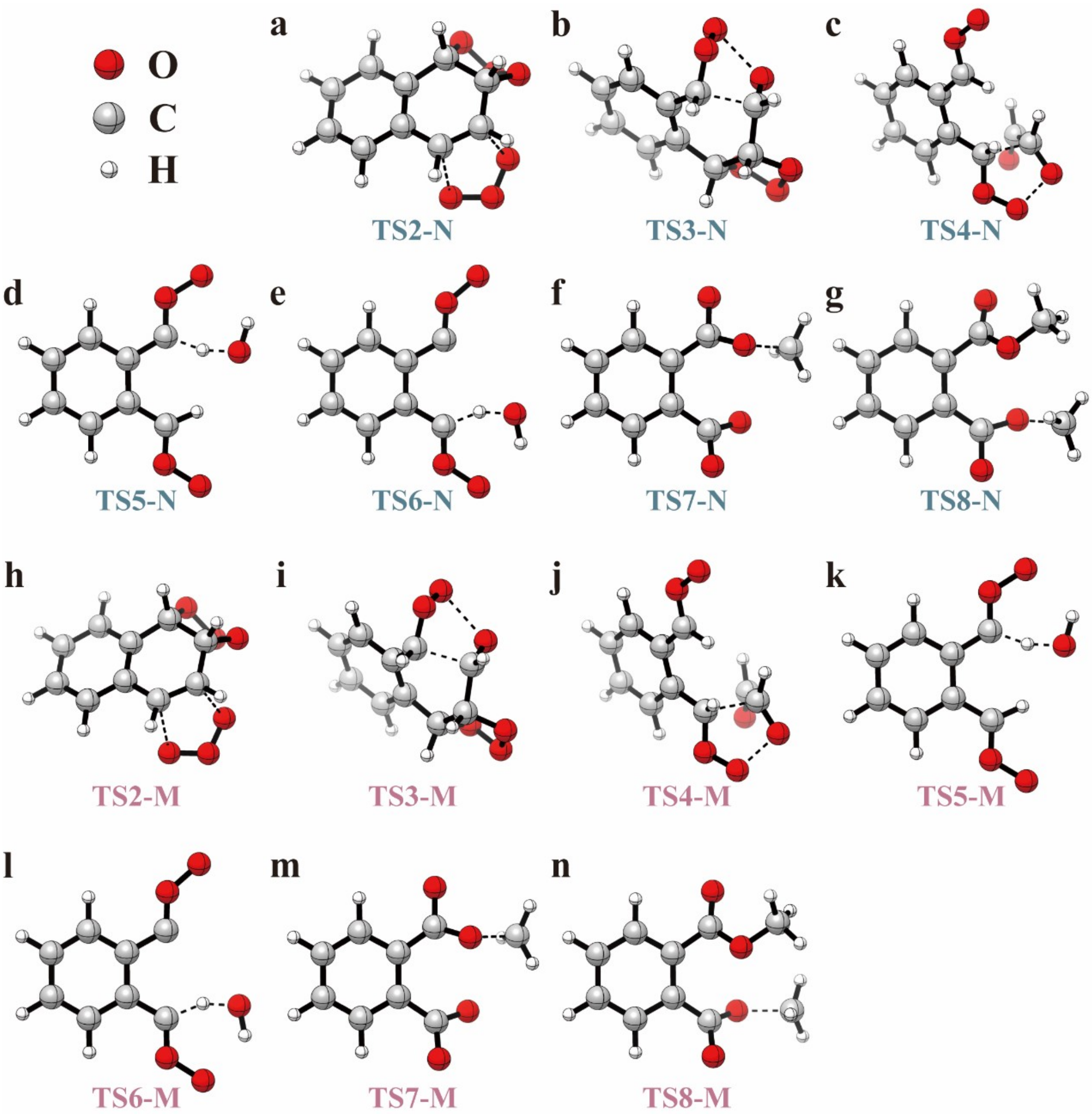


Fig. S19 The optimized structures of transition states

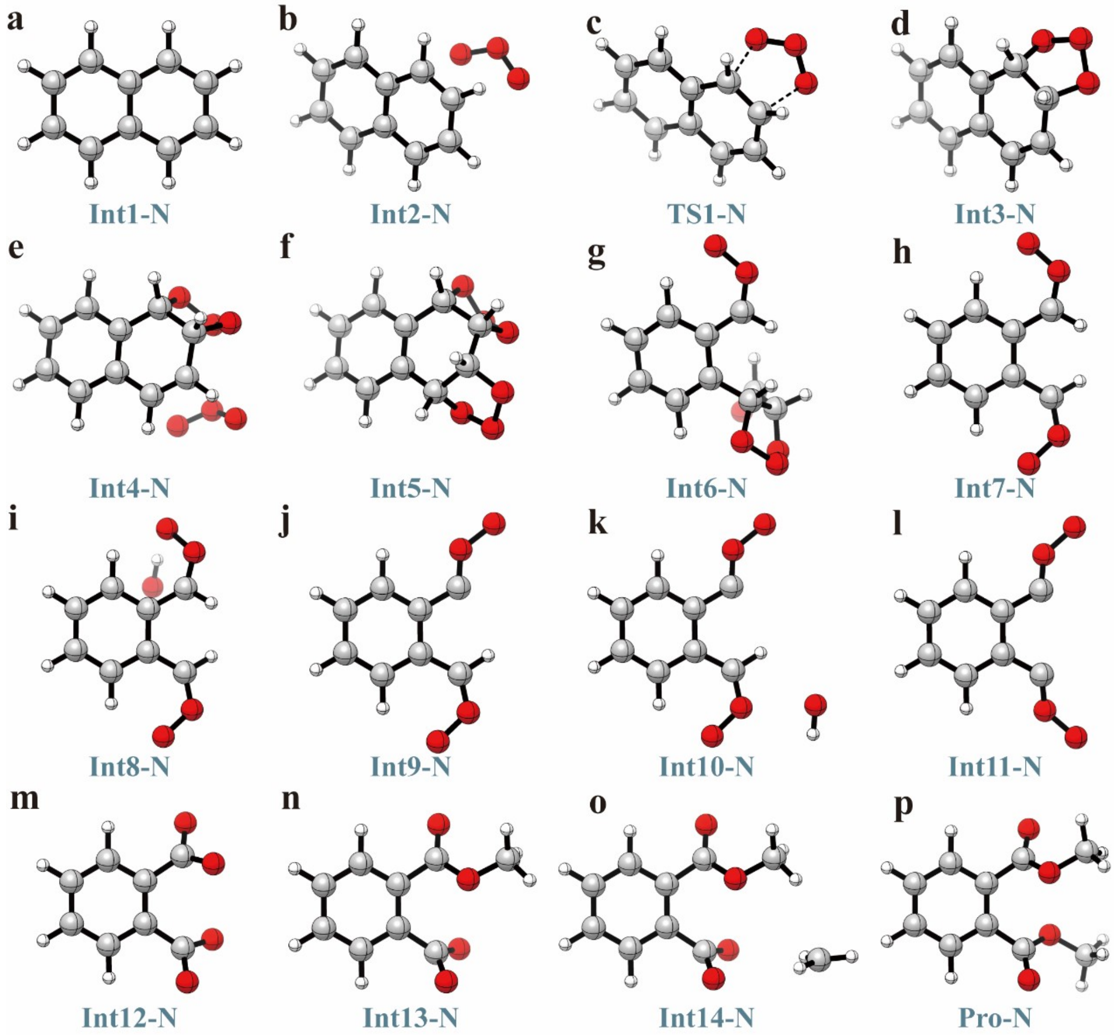


Fig. S20 The optimized structures without microdroplets.

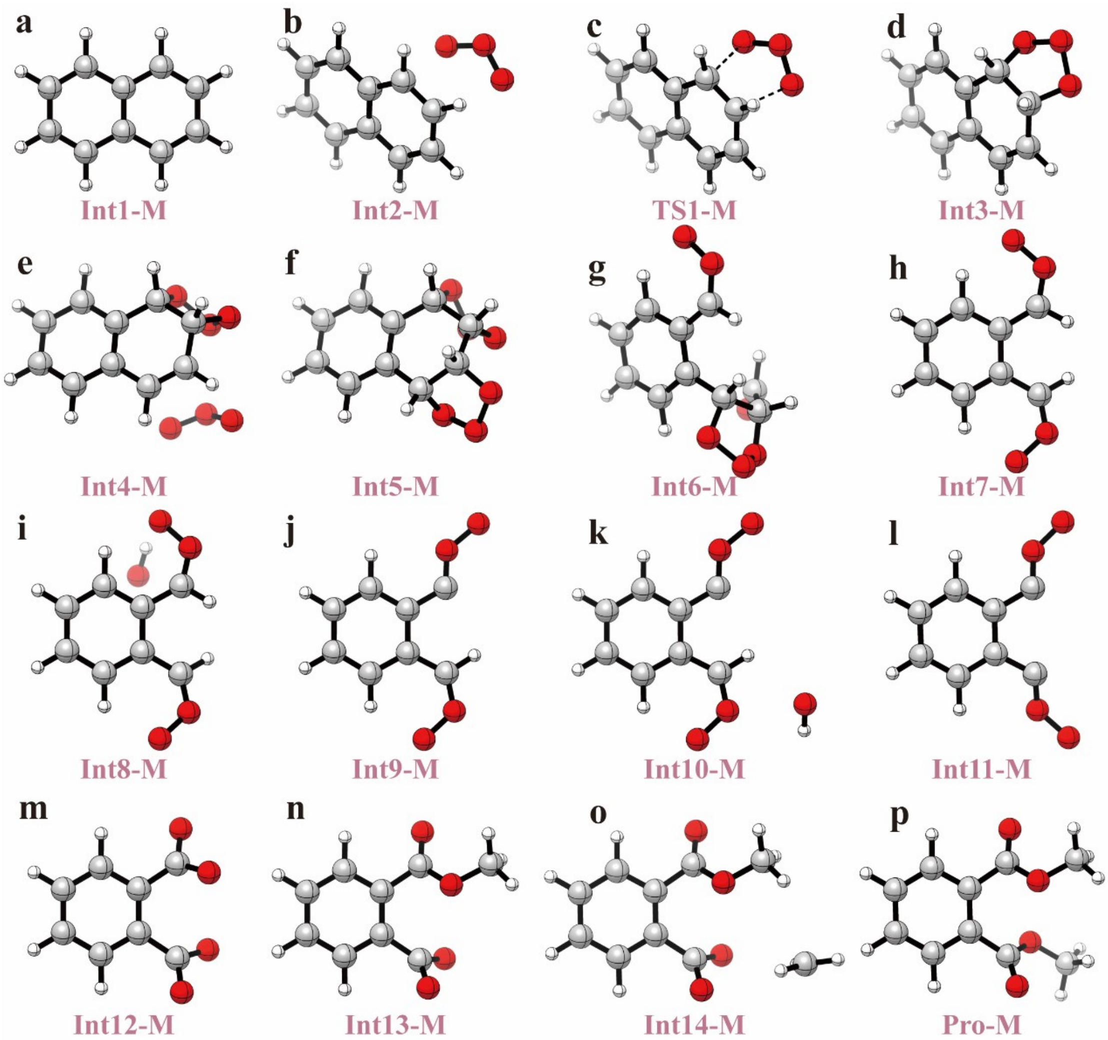


Fig. S21 The optimized structures in microdroplets.

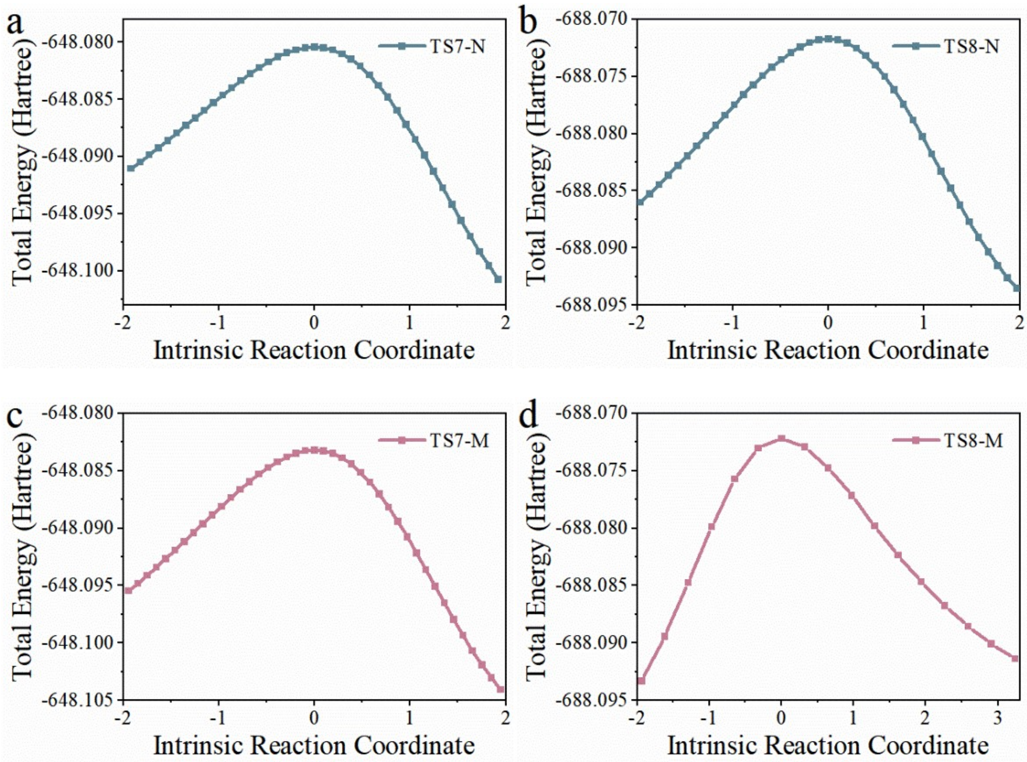
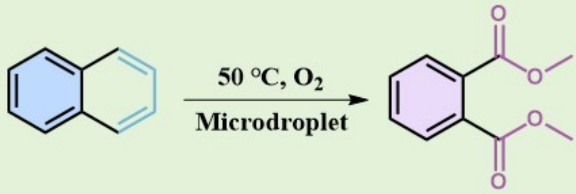


Fig. S22 Total Energy along IRC path: TS7 and TS8 without microdroplets (a) and (b); in microdroplets (c) and (d).

Table S1. A series of microdroplet reactions of naphthalene oxidation carried out under different conditions.



Entry	Naphthalene (mM)	Gas atmosphere	Response modes	Concentration rate of dimethyl phthalate (mM)
1	72.0	O_2	Microdroplet	8.4
2	72.0	Air	Microdroplet	6.8
3	72.0	N_2	Microdroplet	-
4	72.0	O_2	Stir	-
5	72.0	Air	Stir	-
6	72.0	N_2	Stir	-

Reaction condition: 50 °C, CH_3OH:H_2O=1:5.5, reaction time: 4h

Table S2. The energy consumptions and E-factor for the microdroplet spraying process used in naphthalene oxidation.

Electric power		Reaction time	Product molar	Energy consumption	E-factor
Microdroplet	10 W	4 h	0.477 mmol	301.89 kJ/mmol	17.87
	20 W	4 h	0.846 mmol	340.43 kJ/mmol	9.64
	30 W	4 h	0.927 mmol	466.02 kJ/mmol	8.71
Ozonizer	80 W	4h	0.106 mmol	10867.93 kJ/mmol	83.91

The energy consumption (E) was obtained using the following formula:

E=W*t/C W: the power of the experimental device (in kW)

t: reaction time (in h)

C: amount of the products (in mmol)

The E-factor was obtained using the following formula:

$$\text{E-factor} = \frac{Total\ mass\ of\ waste\ generated}{Mass\ of\ isolated\ product}$$

Table S3. A series of microdroplet reactions of naphthalene oxidation carried out under different conditions.

Entry	Addictive	Gas atmosphere	Response modes	Concentration rate of dimethyl phthalate (mM)
1	Catalase	Air	Microdroplet	6.75
2	-	Air	Microdroplet	6.8
3	H_2O_2	N_2	Microdroplet	-
4	-	N_2	Microdroplet	-
5	-	Air	Stir	-
6	-	N_2	Stir	-

The coordinates of the optimized structures

Int1-N			
C	2.428023	0.707201	0.000117
C	1.242005	1.400055	0.00003
C	0.000002	0.71518	-0.000021
C	-0.000002	-0.715179	0.00002
C	1.242006	-1.400055	0.000112
C	2.428022	-0.707201	0.000158
H	-1.239362	2.48476	-0.000143
H	3.370321	1.24257	0.000155
H	1.23936	2.484759	-0.000002
C	-1.242008	1.400056	-0.000112
C	-1.242006	-1.400057	-0.00003
H	1.239362	-2.484759	0.000143
H	3.370321	-1.24257	0.000227
C	-2.428021	-0.707202	-0.000116
C	-2.428021	0.707201	-0.000159
H	-1.239355	-2.48476	0.000002
H	-3.370323	-1.242566	-0.000153
H	-3.370322	1.242567	-0.000228

O_3-N			
O	0	0.428312	0
O	1.0793	-0.214289	0
O	-1.0793	-0.214024	0

Int2-N			
C	-0.967247	1.99597	0.347252
C	0.231663	1.968311	-0.321472
C	1.123404	0.870372	-0.184993
C	0.752169	-0.218987	0.659255
C	-0.504495	-0.173186	1.320142
C	-1.341145	0.919017	1.178691
H	2.649875	1.651027	-1.497964
H	-1.637088	2.839145	0.231625
H	0.51743	2.792217	-0.966513
C	2.36952	0.823315	-0.855634
C	1.638091	-1.31299	0.799644
H	-0.782227	-0.99523	1.970014
H	-2.28208	0.955408	1.713351
C	2.843738	-1.330432	0.136196
C	3.212339	-0.253098	-0.698565
H	1.349556	-2.14202	1.436487
H	3.514543	-2.17374	0.251024
H	4.163306	-0.278494	-1.217654
O	-2.897435	-1.28654	-0.575652
O	-3.410428	-0.128174	-0.691901
O	-1.647328	-1.382543	-0.757881

TS1-N			
C	-1.11404	1.924278	0.393146
C	0.139925	2.010347	-0.123523
C	1.050116	0.897946	-0.090696
C	0.626903	-0.324707	0.48913
C	-0.738358	-0.453572	0.935286
C	-1.602283	0.686368	0.909105
H	2.691084	1.938201	-1.020304
H	-1.771268	2.784591	0.394706
H	0.492211	2.945504	-0.545253
C	2.367159	1.004167	-0.57467
C	1.529115	-1.397203	0.577825
H	-0.976569	-1.269864	1.603634
H	-2.489231	0.684604	1.526074
C	2.821528	-1.270525	0.099625
C	3.240446	-0.064773	-0.482757
H	1.195935	-2.331848	1.014598
H	3.5101	-2.103881	0.171319
H	4.252363	0.029064	-0.858833
O	-2.750087	-1.185401	-0.562671
O	-2.875956	0.115554	-0.698295
O	-1.477419	-1.523944	-0.624131

In3-N			
C	-1.192981	1.86349	0.219303
C	0.098836	1.994173	-0.094675
C	1.049526	0.885464	-0.052564
C	0.61443	-0.406775	0.286168
C	-0.840175	-0.680273	0.541655
C	-1.788614	0.556006	0.630982
H	2.747115	2.090217	-0.582588
H	-1.864896	2.713136	0.185733
H	0.486531	2.965289	-0.384837

C	2.407221	1.09381	-0.322315
C	1.529218	-1.453696	0.356421
H	-0.97297	-1.303506	1.430231
H	-2.22791	0.613277	1.632433
C	2.877804	-1.235971	0.08162
C	3.315036	0.041954	-0.26079
H	1.182406	-2.446344	0.621322
H	3.581442	-2.057809	0.136772
H	4.362536	0.219161	-0.474354
O	-2.768684	-1.190523	-0.445549
O	-2.838757	0.247683	-0.318759
O	-1.357066	-1.399974	-0.595635

In4-N			
C	3.395286	1.207079	-0.129212
C	2.20138	1.547698	0.496882
C	1.173486	0.608349	0.633304
C	1.356509	-0.688195	0.126466
C	2.557672	-1.024452	-0.491835
C	3.576736	-0.083211	-0.62363
H	4.183339	1.944018	-0.229106
H	2.055708	2.549816	0.884581
H	2.695167	-2.02787	-0.880095
H	4.506662	-0.356442	-1.107658
C	0.254238	-1.712703	0.196877
H	0.663382	-2.691312	0.452698
C	-0.069833	0.955293	1.314733
H	-0.182658	1.97677	1.658457
C	-0.950756	-1.370347	1.123155
H	-0.996793	-2.047384	1.97999
C	-1.035985	0.059325	1.562377
H	-1.927445	0.335526	2.11098
O	-1.663407	-1.287195	-0.975454
O	-2.082792	-1.744186	0.316618
O	-0.368591	-1.91655	-1.102827
O	-2.290153	1.583704	-1.044324
O	-3.033126	1.447716	-0.036293
O	-1.28065	2.331995	-0.923288

TS2-N			
C	3.379796	0.835191	-0.191962
C	2.235859	1.394833	0.355969
C	1.09148	0.612849	0.576796
C	1.117628	-0.752189	0.252423
C	2.270844	-1.306131	-0.299536
C	3.395504	-0.519677	-0.528388
H	4.254767	1.449781	-0.365986
H	2.203862	2.451752	0.594082
H	2.284041	-2.359265	-0.555546
H	4.283848	-0.962112	-0.963136
C	-0.049194	-1.661522	0.553812
H	0.259079	-2.418103	1.278906
C	-0.120935	1.227123	1.086919
H	-0.041207	2.211892	1.527219
C	-1.365827	-0.969082	1.032245
H	-1.679179	-1.387224	1.992293
C	-1.312786	0.532485	1.179371
H	-2.139581	0.970475	1.722283
O	-1.573593	-1.645998	-1.092778
O	-2.346951	-1.449178	0.105116
O	-0.475288	-2.426926	-0.58604
O	-1.892891	2.368049	-0.68932
O	-2.269097	1.129891	-0.628833
O	-0.602162	2.484103	-0.775145

Int5-N			
C	-3.197961	-1.389903	-0.266744
C	-1.873037	-1.789463	-0.164139
C	-0.873858	-0.868285	0.167349
C	-1.211596	0.465956	0.40606
C	-2.552164	0.855414	0.322124
C	-3.53928	-0.060241	-0.015682
H	-3.963199	-2.109619	-0.531127
H	-1.599207	-2.822997	-0.343664
H	-2.814441	1.891616	0.503219
H	-4.572386	0.259152	-0.083239
C	-0.188047	1.538273	0.700172
H	-0.45377	2.106327	1.593168
C	0.532336	-1.358494	0.311619
H	0.554221	-2.340665	0.793824
C	1.294163	1.073588	0.737762
H	1.854833	1.660354	1.468045
C	1.49566	-0.418065	1.040769
H	1.432725	-0.582337	2.121915
O	-0.157112	2.509191	-0.355236

O	1.811179	1.460351	-0.542488
O	0.638793	1.815316	-1.322356
O	2.778847	-0.832801	0.600484
O	1.195261	-1.471223	-0.955869
O	2.513524	-1.775147	-0.544271

TS3-N			
C	-2.512395	-2.202278	-0.270621
C	-1.138808	-2.206046	-0.076363
C	-0.467172	-1.033357	0.28327
C	-1.187515	0.148255	0.457425
C	-2.575175	0.145123	0.266858
C	-3.233452	-1.021508	-0.091869
H	-3.02085	-3.114308	-0.558696
H	-0.56985	-3.117717	-0.213968
H	-3.132969	1.065119	0.387616
H	-4.306949	-1.009282	-0.236458
C	-0.552059	1.43455	0.873704
H	-0.432383	1.635194	1.937853
C	1.013533	-1.102034	0.495894
H	1.250902	-1.795115	1.310986
C	1.169102	1.498372	0.108759
H	1.57233	2.404842	0.594539
C	1.756493	0.216937	0.759434
H	1.867151	0.391811	1.835206
O	-0.963603	2.556996	0.260128
O	0.923708	1.541555	-1.128873
O	-1.059954	2.383272	-1.046685
O	3.048077	0.009017	0.193367
O	1.669715	-1.57463	-0.686548
O	3.024219	-1.382287	-0.328393

Int6-N			
C	-0.768631	2.679207	-0.329953
C	0.211341	1.708776	-0.538281
C	-0.110611	0.357658	-0.522984
C	-1.456935	-0.039219	-0.265905
C	-2.433796	0.960922	-0.050525
C	-2.085597	2.303687	-0.089635
H	-0.49308	3.7268	-0.351398
H	1.235506	2.00323	-0.721208
H	-3.444123	0.64135	0.147575
H	-2.847066	3.055949	0.075513
C	-1.773034	-1.437333	-0.217809
H	-1.023188	-2.186832	-0.436774
C	1.006963	-0.641461	-0.710969
H	0.664395	-1.594403	-1.111802
C	1.432196	-0.150125	1.814536
H	0.441902	-0.476303	2.194055
C	1.883835	-0.924768	0.583792
H	1.841894	-1.997977	0.813149
O	-2.874468	-2.020939	0.063277
O	2.064668	0.714551	2.351586
O	-3.997614	-1.32147	0.387908
O	3.18736	-0.533291	0.203154
O	1.966488	-0.090756	-1.611928
O	3.177238	-0.75758	-1.224338

TS4-N			
C	-0.710763	2.913953	-0.265823
C	0.221658	1.919606	-0.524535
C	-0.150951	0.570724	-0.506116
C	-1.491603	0.223756	-0.195484
C	-2.419767	1.249837	0.073725
C	-2.033761	2.577223	0.035966
H	-0.405353	3.952637	-0.290038
H	1.249969	2.179868	-0.734345
H	-3.441293	0.981876	0.308851
H	-2.758934	3.354223	0.243918
C	-1.905824	-1.152716	-0.139809
H	-1.270565	-2.001257	-0.372927
C	0.867712	-0.466032	-0.752219
H	0.557879	-1.43662	-1.124678
C	1.711916	0.117316	1.709083
H	0.858773	0.140175	2.422441
C	1.721247	-1.11036	0.801051
H	0.970757	-1.870393	1.081639
O	-3.093429	-1.442059	0.204724
O	2.528954	0.993383	1.666366
O	-3.451034	-2.756142	0.240786
O	2.855587	-1.533588	0.372163
O	1.987813	-0.023624	-1.361629
O	2.844559	-1.033012	-1.491148

Int7-N			
C	0.694644	2.401682	-0.006475
C	1.402008	1.202156	-0.005082
C	0.723333	-0.02917	0.011835
C	-0.723333	-0.029176	-0.011823
C	-1.402018	1.202144	0.005088
C	-0.694665	2.401676	0.006481
H	1.241306	3.337	-0.010558
H	2.479934	1.18374	-0.004032
H	-2.479944	1.18372	0.004033
H	-1.241335	3.33699	0.010563
C	-1.430349	-1.269508	-0.141574
H	-0.910317	-2.19681	-0.343249
C	1.430359	-1.269496	0.141602
H	0.910337	-2.196794	0.343314
O	-2.688024	-1.501288	-0.10089
O	-3.597352	-0.518076	0.127001
O	2.688034	-1.501274	0.100892
O	3.597359	-0.518072	-0.127051

Int8-N			
C	-0.920223	2.427276	0.06138
C	-1.599414	1.210832	0.021487
C	-0.896443	0.002812	0.153509
C	0.526294	0.045461	0.367528
C	1.183803	1.286884	0.372356
C	0.458043	2.466387	0.232408
H	-1.480004	3.347427	-0.054873
H	-2.665989	1.165343	-0.128589
H	2.253302	1.304034	0.512
H	0.979828	3.415125	0.255506
C	1.218148	-1.160813	0.734332
H	0.682541	-2.000856	1.16326
C	-1.520178	-1.272474	-0.047812
H	-0.926372	-2.165709	-0.198773
O	2.463224	-1.420064	0.680964
O	3.336441	-0.519465	0.112229
O	-2.762009	-1.560793	-0.142253
O	-3.725322	-0.614276	-0.012423
O	1.676609	-0.231423	-2.054085
H	2.544969	-0.335376	-1.595115

TS5-N			
C	0.790198	2.985294	-0.000005
C	-0.362073	2.222867	-0.000002
C	-0.28911	0.814908	0.000001
C	0.983312	0.17436	0.000001
C	2.139899	0.978181	-0.000003
C	2.043697	2.35777	-0.000006
H	-1.335614	2.695323	-0.000003
H	3.109564	0.499164	-0.000003
H	2.946735	2.955909	-0.000008
H	0.722317	4.066062	-0.000008
C	1.102098	-1.262878	0.000004
H	0.2745	-1.966679	0.000005
C	-1.49106	0.029319	0.000004
H	-1.621712	-1.258744	-0.000007
O	2.272585	-1.76322	0.000005
O	-2.626238	0.570456	0.000014
O	-2.086791	-2.35821	-0.000026
H	-3.047402	-2.199396	-0.000019
O	-3.786007	-0.163714	0.000009
O	2.407681	-3.109133	0.000008

Int9-N			
C	0.071126	2.649639	-0.000462
C	1.040221	1.655403	-0.001533
C	0.662779	0.304968	-0.001333
C	-0.722766	-0.051332	-0.000756
C	-1.684205	0.978257	0.000561
C	-1.281872	2.309002	0.00064
H	2.092529	1.908543	-0.002498
H	-2.725498	0.699101	0.001397
H	-2.034289	3.088185	0.001369
H	0.371924	3.69043	-0.000505
C	-1.048565	-1.449214	-0.001689
H	-0.254537	-2.188626	-0.00386
C	1.663063	-0.732718	-0.00339
O	-2.194096	-2.008991	-0.000554
O	2.876135	-0.505327	0.006211
O	3.955179	-1.350719	-0.001266
O	-3.34332	-1.282673	0.002093

Int10-N			

C	-0.509167	-2.907037	0.002039
C	0.541876	-1.997473	0.000909
C	0.279987	-0.613339	-0.002179
C	-1.08054	-0.172273	-0.003083
C	-2.121248	-1.111576	-0.002545
C	-1.834075	-2.470229	0.000306
H	-0.29054	-3.967867	0.004123
H	1.570869	-2.319458	0.002185
H	-3.145958	-0.763266	-0.004259
H	-2.64522	-3.188431	0.000999
C	-1.371367	1.240726	-0.008044
C	1.302543	0.392716	-0.004517
H	1.044441	1.446238	-0.009101
O	-2.52148	1.688721	0.012354
O	-2.994637	2.972569	-0.002573
O	2.568287	0.242219	-0.002386
O	3.157719	-0.983025	0.003571
O	3.294211	2.628038	0.002522
H	4.185555	2.23551	0.000831

TS6-N			
C	2.055597	2.349972	0.092585
C	2.158223	0.968448	0.072358
C	0.99857	0.174727	0.019329
C	-0.274925	0.799206	-0.002997
C	-0.355331	2.20291	0.019022
C	0.799138	2.966868	0.064506
H	3.126135	0.48492	0.094983
H	-1.328871	2.674957	0.005272
H	0.726606	4.047352	0.083063
H	2.954117	2.953693	0.131961
C	-1.466879	-0.013417	-0.033991
H	-1.574741	-1.295384	0.189677
C	1.080924	-1.267377	0.005117
O	-2.5847	0.525638	-0.23445
O	2.156279	-1.85114	-0.170725
O	-2.154503	-2.310232	0.419332
H	-3.091244	-2.065026	0.290233
O	2.492442	-3.16923	-0.115055
O	-3.757506	-0.181102	-0.175448

Int11-N			
C	0.700044	2.686663	-0.024944
C	1.403903	1.493291	0.021868
C	0.708132	0.272931	0.069387
C	-0.708113	0.272732	0.069084
C	-1.404174	1.492952	0.021047
C	-0.700607	2.686491	-0.025419
H	1.23893	3.625638	-0.061948
H	2.486213	1.486272	0.024799
H	-2.486485	1.485634	0.023362
H	-1.239706	3.625328	-0.062812
C	-1.393863	-0.99208	0.163005
C	1.394016	-0.991882	0.162955
O	-2.573801	-1.114186	-0.194624
O	-3.466869	-2.120493	0.028236
O	2.574116	-1.113755	-0.194125
O	3.467182	-2.120248	0.027351

Int12-N			
C	2.650899	-0.695943	0.000507
C	1.4456	-1.393439	0.008683
C	0.23241	-0.703358	0.009255
C	0.232371	0.703363	-0.009269
C	1.445523	1.393513	-0.00869
C	2.65086	0.696083	-0.000502
H	3.587002	-1.240686	0.003129
H	1.434834	-2.475851	0.03367
H	1.434696	2.475924	-0.033668
H	3.586933	1.240878	-0.003113
C	-1.003284	1.514714	-0.117441
C	-1.003213	-1.514759	0.117424
O	-1.124303	2.639732	0.431675
O	-1.12414	-2.639829	-0.431612
O	-1.997662	-1.20274	0.815559
O	-1.997702	1.202674	-0.815599

Int13-N			
C	2.661111	-1.44739	0.098154
C	1.304563	-1.745982	0.00287
C	0.355936	-0.72614	-0.040357
C	0.784754	0.613369	-0.014383
C	2.14873	0.907049	0.088452
C	3.083574	-0.120605	0.148746

H	3.386962	-2.250631	0.137217
H	0.959852	-2.771672	-0.028644
H	2.466718	1.942177	0.104298
H	4.138188	0.1142	0.225886
C	-0.134441	1.765525	-0.181948
C	-1.084206	-1.126366	-0.070339
O	-0.173063	2.722268	0.630027
O	-1.487063	-2.172499	-0.519043
O	-0.863692	1.926237	-1.190706
O	-1.862978	-0.19643	0.500327
C	-3.283515	-0.428467	0.448097
H	-3.732178	0.429137	0.942257
H	-3.611669	-0.492034	-0.589621
H	-3.532535	-1.353745	0.968016

TS7-N			
C	-3.112049	-0.000987	0.069268
C	-2.130204	0.979247	-0.003862
C	-0.773395	0.640456	-0.02684
C	-0.387791	-0.728237	-0.0208
C	-1.401769	-1.707238	0.074018
C	-2.737518	-1.347978	0.125731
H	-4.157337	0.279325	0.098266
H	-2.402411	2.027517	-0.009689
H	-1.119747	-2.752645	0.069175
H	-3.495606	-2.118973	0.194402
C	0.956037	-1.196652	-0.227648
C	0.179258	1.754178	0.050383
O	1.334455	-2.404361	0.090792
O	-0.059567	2.897742	-0.44074
O	1.275449	1.735934	0.66406
O	1.930821	-0.573361	-0.770433
C	3.484614	-0.129952	0.309554
H	3.630045	0.868465	-0.073543
H	3.090489	-0.21564	1.312673
H	4.142219	-0.912701	-0.039534

Int14-N			
C	3.431241	-0.244298	0.225617
C	2.348001	-1.110193	0.102658
C	1.052409	-0.612622	-0.02376
C	0.851244	0.779468	-0.052223
C	1.943142	1.644793	0.079977
C	3.228578	1.13418	0.221882
H	4.431948	-0.646148	0.328987
H	2.487216	-2.183633	0.113219
H	1.7757	2.71446	0.055008
H	4.069	1.810341	0.320868
C	-0.467197	1.412054	-0.300866
C	-0.061955	-1.608662	-0.077267
O	-0.964029	2.258646	0.482748
O	0.071579	-2.750704	-0.44707
O	-1.13154	1.240521	-1.351023
C	-4.291007	1.173016	0.333154
H	-5.341588	0.924436	0.39297
H	-3.767312	1.536464	1.205722
H	-3.770526	1.130732	-0.612717
O	-1.210076	-1.086866	0.372799
C	-2.374221	-1.934556	0.302798
H	-3.199742	-1.310639	0.635897
H	-2.530245	-2.267174	-0.723478
H	-2.24332	-2.800704	0.952076

TS8-N			
C	-3.274432	-0.472177	0.276979
C	-2.142334	-1.262638	0.202253
C	-0.863024	-0.691195	-0.006055
C	-0.762816	0.722361	-0.108327
C	-1.925233	1.49251	-0.081066
C	-3.174818	0.91321	0.116965
H	-4.241641	-0.934639	0.434114
H	-2.226951	-2.340585	0.261453
H	-1.827719	2.564931	-0.193551
H	-4.060838	1.534929	0.150412
C	0.509479	1.490259	-0.184098
C	0.217592	-1.60778	-0.237544
O	0.655277	2.503094	-0.8284
O	0.164966	-2.852701	0.172943
O	1.308663	-1.406475	-0.880078
C	2.930065	-1.587346	0.067436
H	2.649196	-1.31131	1.07409
H	3.144191	-2.630771	-0.114259
H	3.511556	-0.86903	-0.492187
O	1.467257	0.990194	0.626011
C	2.698325	1.734089	0.648323

H	3.349315	1.202204	1.338201
H	3.138141	1.772437	-0.348966
H	2.518627	2.751185	0.997688

Pro-N			
C	-3.217347	-0.686557	0.11487
C	-2.011781	-1.372914	0.219149
C	-0.797934	-0.695158	0.097668
C	-0.797737	0.69523	-0.097812
C	-2.011382	1.373359	-0.219135
C	-3.217148	0.687371	-0.114677
H	-4.153386	-1.224727	0.204732
H	-1.995041	-2.443148	0.382277
H	-1.994362	2.443586	-0.382284
H	-4.153032	1.225833	-0.204415
C	0.445841	1.522407	-0.12435
C	0.445365	-1.522719	0.124061
O	0.623959	2.465789	-0.856473
O	0.622853	-2.466828	0.8554
O	1.321478	-1.13364	-0.82251
C	2.572469	-1.841528	-0.843783
H	3.137817	-1.406043	-1.664273
H	3.096812	-1.705727	0.103438
H	2.405798	-2.905928	-1.011656
O	1.321329	1.133925	0.823065
C	2.572573	1.841378	0.844356
H	3.137369	1.40641	1.665502
H	3.097354	1.704585	-0.10248
H	2.406209	2.905985	1.011221

Int1-M			
C	2.428441	0.707365	0.001356
C	1.242269	1.400272	0.006632
C	0	0.715174	0.011332
C	-0.000001	-0.715173	0.011374
C	1.242269	-1.400271	0.006714
C	2.428441	-0.707364	0.001397
H	-1.23966	2.484991	-0.001921
H	3.370762	1.242677	-0.011585
H	1.239659	2.484991	-0.001781
C	-1.24227	1.400272	0.006492
C	-1.242269	-1.400272	0.006574
H	1.23966	-2.48499	-0.001635
H	3.370763	-1.242676	-0.011512
C	-2.42844	-0.707366	0.001122
C	-2.42844	0.707365	0.001081
H	-1.239658	-2.484991	-0.001775
H	-3.370761	-1.242676	-0.011895
H	-3.370761	1.242675	-0.011968

O_3-M			
O	-0.001935	0.428711	0
O	1.080053	-0.215064	0
O	-1.078117	-0.213648	0

Int2-M			
C	-0.971068	2.003562	0.366257
C	0.221937	1.973591	-0.310862
C	1.11282	0.874613	-0.177043
C	0.747808	-0.210028	0.676207
C	-0.502004	-0.159646	1.34928
C	-1.340019	0.92846	1.204958
H	2.624058	1.642064	-1.514465
H	-1.64382	2.844336	0.250332
H	0.501153	2.793248	-0.964159
C	2.350972	0.819132	-0.862621
C	1.632353	-1.306857	0.810179
H	-0.777197	-0.980152	2.002255
H	-2.279205	0.966618	1.742742
C	2.828824	-1.332778	0.131655
C	3.191078	-0.259943	-0.712735
H	1.346053	-2.133317	1.451426
H	3.495108	-2.181026	0.23845
H	4.133459	-0.292955	-1.247557
O	-2.86427	-1.282247	-0.624117
O	-3.291478	-0.098833	-0.765606
O	-1.620401	-1.468494	-0.769123

TS1-M			
C	-1.115137	1.920894	0.39628
C	0.136683	2.005778	-0.125976

C	1.048923	0.895223	-0.092088
C	0.627745	-0.326363	0.491188
C	-0.739909	-0.45827	0.932546
C	-1.603257	0.683037	0.913524
H	2.686329	1.933827	-1.029965
H	-1.7737	2.780471	0.396369
H	0.486358	2.939393	-0.554026
C	2.365217	1.001609	-0.577898
C	1.531604	-1.396832	0.584217
H	-0.978837	-1.278343	1.596154
H	-2.486944	0.68056	1.53512
C	2.824154	-1.269317	0.105906
C	3.240331	-0.065652	-0.482446
H	1.200908	-2.331018	1.023486
H	3.513511	-2.101552	0.180238
H	4.251319	0.026562	-0.861485
O	-2.743424	-1.175114	-0.570946
O	-2.882284	0.127612	-0.688212
O	-1.467917	-1.497598	-0.638673

In3-M			
C	-1.192856	1.868929	0.227238
C	0.102842	2.001547	-0.068882
C	1.050625	0.889855	-0.035084
C	0.615075	-0.402518	0.301998
C	-0.838412	-0.675875	0.570047
C	-1.797533	0.556428	0.607945
H	2.745035	2.090541	-0.582685
H	-1.863379	2.719596	0.194478
H	0.495051	2.975677	-0.342602
C	2.406107	1.094088	-0.320835
C	1.527089	-1.453049	0.355337
H	-0.965489	-1.261486	1.484915
H	-2.28927	0.611351	1.584414
C	2.87267	-1.239637	0.063578
C	3.310485	0.038543	-0.277708
H	1.178496	-2.445749	0.61735
H	3.5725	-2.065926	0.102427
H	4.355455	0.212609	-0.507232
O	-2.754087	-1.199084	-0.449295
O	-2.790299	0.239682	-0.395631
O	-1.340057	-1.446734	-0.539198

In4-M			
C	3.396803	1.207322	-0.123146
C	2.205036	1.545032	0.509061
C	1.177517	0.605443	0.644002
C	1.35815	-0.688604	0.129992
C	2.556758	-1.021891	-0.494854
C	3.575933	-0.080295	-0.624848
H	4.182706	1.945885	-0.227506
H	2.058685	2.547076	0.897042
H	2.691	-2.021403	-0.893971
H	4.501463	-0.349554	-1.119145
C	0.253732	-1.711466	0.195643
H	0.662837	-2.693225	0.439696
C	-0.06682	0.950559	1.325162
H	-0.184458	1.974471	1.66063
C	-0.945215	-1.375126	1.131448
H	-0.983312	-2.055016	1.986641
C	-1.031623	0.05429	1.571784
H	-1.930564	0.332285	2.107623
O	-1.672973	-1.279846	-0.959581
O	-2.081671	-1.748468	0.33279
O	-0.377698	-1.902838	-1.100993
O	-2.293536	1.578033	-1.063274
O	-3.048544	1.484862	-0.059276
O	-1.266829	2.299917	-0.951527

TS2-M			
C	3.377346	0.833408	-0.201506
C	2.232108	1.39454	0.341392
C	1.09052	0.610495	0.571542
C	1.120093	-0.757506	0.258148
C	2.276145	-1.313501	-0.285591
C	3.39834	-0.525629	-0.521517
H	4.250544	1.44849	-0.383195
H	2.195279	2.453861	0.568677
H	2.294167	-2.369248	-0.529586
H	4.288986	-0.971076	-0.948141
C	-0.047841	-1.667351	0.556063
H	0.258182	-2.426535	1.279066
C	-0.118893	1.222149	1.087516
H	-0.039082	2.208395	1.524452
C	-1.36596	-0.974283	1.029685
H	-1.686918	-1.395432	1.985811

C	-1.309903	0.527266	1.182332
H	-2.136864	0.965185	1.725104
O	-1.557624	-1.634688	-1.100453
O	-2.341451	-1.442416	0.092464
O	-0.469671	-2.424784	-0.589322
O	-1.911487	2.383878	-0.672417
O	-2.266664	1.139917	-0.624768
O	-0.621334	2.525882	-0.764989

Int5-M			
C	-3.199614	-1.390727	-0.260902
C	-1.87361	-1.788936	-0.166284
C	-0.873866	-0.867374	0.162325
C	-1.212049	0.465954	0.406562
C	-2.553579	0.853817	0.330615
C	-3.541377	-0.062255	-0.004237
H	-3.964491	-2.109372	-0.52894
H	-1.599085	-2.820653	-0.354895
H	-2.815642	1.890356	0.510543
H	-4.574546	0.256992	-0.07111
C	-0.188108	1.539868	0.692547
H	-0.456375	2.116104	1.579656
C	0.532891	-1.356504	0.304469
H	0.554885	-2.34162	0.781099
C	1.294107	1.073773	0.739028
H	1.85137	1.658971	1.473575
C	1.492114	-0.41844	1.042643
H	1.418838	-0.583659	2.123348
O	-0.153264	2.50179	-0.369854
O	1.819353	1.46158	-0.535578
O	0.650754	1.802936	-1.3265
O	2.776904	-0.83562	0.614207
O	1.202931	-1.460595	-0.958679
O	2.51694	-1.770088	-0.541942

TS3-M			
C	-2.519355	-2.208322	-0.250899
C	-1.142931	-2.206731	-0.07699
C	-0.468606	-1.030538	0.265702
C	-1.189725	0.150757	0.442108
C	-2.580451	0.142127	0.272885
C	-3.240942	-1.028659	-0.068701
H	-3.030567	-3.123724	-0.522376
H	-0.574543	-3.119107	-0.213548
H	-3.140926	1.059519	0.401738
H	-4.316836	-1.021073	-0.192879
C	-0.562568	1.442501	0.853424
H	-0.47101	1.659438	1.917132
C	1.012924	-1.099719	0.468859
H	1.256655	-1.821949	1.256102
C	1.186184	1.500273	0.128213
H	1.5757	2.400722	0.6372
C	1.750915	0.210265	0.777078
H	1.831007	0.364561	1.858577
O	-0.955641	2.555785	0.213696
O	0.977193	1.558469	-1.114838
O	-1.018351	2.367724	-1.090757
O	3.061148	0.003097	0.252799
O	1.675082	-1.524296	-0.730358
O	3.027742	-1.358641	-0.357604

Int6-M			
C	-0.722115	2.643123	-0.305043
C	0.231475	1.648433	-0.509124
C	-0.12372	0.304035	-0.502255
C	-1.482922	-0.058763	-0.270028
C	-2.434911	0.966885	-0.059847
C	-2.051512	2.299806	-0.083691
H	-0.418128	3.68316	-0.314441
H	1.265603	1.914778	-0.679535
H	-3.456172	0.672554	0.120141
H	-2.796362	3.069607	0.077777
C	-1.850249	-1.44723	-0.259811
H	-1.131857	-2.220352	-0.499833
C	0.988337	-0.706452	-0.672203
H	0.637852	-1.698547	-0.94962
C	1.444237	-0.14933	1.833245
H	0.511574	-0.599835	2.230292
C	1.954329	-0.841504	0.580647
H	2.101273	-1.906199	0.803135
O	-2.976888	-1.990119	0.000053
O	1.981812	0.777803	2.371544
O	-4.069935	-1.256473	0.342692
O	3.157579	-0.25141	0.133472
O	1.870015	-0.221809	-1.690503

O	3.176329	-0.652487	-1.246028

TS4-M			
C	-0.716264	2.918374	-0.264263
C	0.220004	1.926692	-0.519766
C	-0.149619	0.577159	-0.504269
C	-1.490101	0.225568	-0.197182
C	-2.42214	1.248708	0.068971
C	-2.039529	2.577473	0.031702
H	-0.415321	3.958352	-0.288847
H	1.247855	2.189872	-0.728766
H	-3.444394	0.978979	0.299142
H	-2.768677	3.351991	0.234528
C	-1.895821	-1.153177	-0.138668
H	-1.260886	-1.997907	-0.385723
C	0.869685	-0.459776	-0.749711
H	0.556423	-1.422902	-1.138996
C	1.716662	0.111722	1.704187
H	0.835362	0.181912	2.378091
C	1.700031	-1.112401	0.791572
H	0.932787	-1.855741	1.070146
O	-3.074205	-1.452712	0.229524
O	2.584979	0.939181	1.703648
O	-3.416984	-2.765896	0.271816
O	2.828765	-1.564835	0.37076
O	1.997652	-0.01758	-1.351245
O	2.847284	-1.034282	-1.484689

Int7-M			
C	0.694504	2.398924	-0.002829
C	1.400618	1.199392	0.000185
C	0.7232	-0.033278	0.010887
C	-0.723224	-0.03327	-0.010883
C	-1.400608	1.199423	-0.000188
C	-0.694461	2.398938	0.00282
H	1.242524	3.333643	-0.003622
H	2.478396	1.179521	0.003898
H	-2.478384	1.179585	-0.003906
H	-1.242458	3.333671	0.003607
C	-1.437924	-1.272477	-0.12074
H	-0.925986	-2.210496	-0.290488
C	1.437909	-1.272473	0.120741
H	0.926005	-2.210513	0.290477
O	-2.698124	-1.490304	-0.087064
O	-3.601535	-0.495432	0.103428
O	2.698121	-1.490205	0.087093
O	3.601405	-0.495207	-0.103341

Int8-M			
C	-0.932232	2.412355	0.015074
C	-1.62114	1.200205	0.009615
C	-0.92544	-0.010412	0.139918
C	0.501332	0.020408	0.332842
C	1.165822	1.260161	0.326373
C	0.447142	2.442782	0.172784
H	-1.486158	3.334206	-0.114752
H	-2.691501	1.16426	-0.11621
H	2.233846	1.27176	0.469781
H	0.976991	3.387253	0.173253
C	1.178779	-1.198914	0.664967
H	0.620717	-2.071407	0.98544
C	-1.580577	-1.276107	-0.043465
H	-1.020845	-2.166137	-0.304822
O	2.426816	-1.456833	0.694381
O	3.347446	-0.518892	0.289302
O	-2.827885	-1.547822	0.007491
O	-3.750323	-0.599228	0.311283
O	1.962713	-0.025745	-2.026082
H	2.801747	-0.23156	-1.554137

TS5-M			
C	2.438057	-1.241446	0.026883
C	1.107204	-1.612997	0.025841
C	0.091154	-0.635742	0.013837
C	0.440205	0.745184	-0.000231
C	1.804905	1.092978	-0.001066
C	2.784542	0.116714	0.012576
H	0.826698	-2.658145	0.031173
H	2.077886	2.139374	-0.019449
H	3.827928	0.407507	0.005557
H	3.210458	-2.000396	0.032407
C	-0.568521	1.776221	-0.00095
H	-1.64103	1.612966	-0.059959
C	-1.289924	-1.028785	0.025582

H	-2.347744	-0.286519	-0.05062
O	-0.181725	2.985877	0.082677
O	-1.624762	-2.237562	0.115979
O	-3.483037	0.08325	-0.068605
H	-3.993183	-0.745801	-0.085048
O	-2.939149	-2.633499	0.118046
O	-1.110228	3.969868	0.093343

Int9-M			
C	0.07731	2.64129	-0.000353
C	1.041812	1.643473	-0.001517
C	0.661199	0.293669	-0.001374
C	-0.724181	-0.058351	-0.000796
C	-1.682129	0.975523	0.000463
C	-1.276593	2.304662	0.000651
H	2.095202	1.891869	-0.00247
H	-2.723911	0.698474	0.001189
H	-2.027832	3.085198	0.0015
H	0.382238	3.68107	-0.000325
C	-1.059823	-1.455222	-0.001495
H	-0.274052	-2.2032	-0.003295
C	1.664569	-0.745446	-0.00353
O	-2.212246	-2.000807	-0.000509
O	2.873013	-0.488454	0.005701
O	3.980356	-1.287157	-0.001159
O	-3.351126	-1.262661	0.001745

Int10-M			
C	0.769842	2.644617	0.024913
C	-0.405289	1.902863	0.059999
C	-0.355212	0.495915	0.01811
C	0.922831	-0.143189	-0.038091
C	2.092432	0.628814	-0.074391
C	2.012899	2.014866	-0.044361
H	0.713267	3.726057	0.046835
H	-1.372923	2.375513	0.113442
H	3.051743	0.130629	-0.127792
H	2.921663	2.603844	-0.07629
C	1.000106	-1.58291	-0.05864
C	-1.516418	-0.346446	0.00786
H	-1.425099	-1.419834	-0.119805
O	2.055681	-2.200707	0.109045

O	2.337604	-3.539245	0.055352
O	-2.74222	-0.014503	0.123435
O	-3.130366	1.275941	0.306997
O	-3.706194	-2.358658	0.026266
H	-4.442068	-1.93229	-0.449387

TS6-M			
C	2.442359	-1.23671	-0.036367
C	1.111756	-1.624371	-0.014443
C	0.094696	-0.655234	0.037272
C	0.442143	0.720107	0.058107
C	1.798528	1.09107	0.034605
C	2.785256	0.120502	-0.010756
H	0.841834	-2.672263	-0.034811
H	2.057092	2.141673	0.047329
H	3.827396	0.414947	-0.030556
H	3.2193	-1.990474	-0.074728
C	-0.597744	1.719187	0.089849
H	-1.872193	1.546249	-0.121996
C	-1.30381	-1.023722	0.053272
O	-0.302972	2.925575	0.284422
O	-1.647264	-2.201542	0.21635
O	-2.987921	1.910527	-0.338728
H	-2.923333	2.876956	-0.205668
O	-2.854059	-2.813238	0.177377
O	-1.246912	3.927505	0.226691

Int11-M			
C	0.70003	2.674954	-0.026211
C	1.402245	1.481302	0.020855
C	0.70738	0.25992	0.06849
C	-0.70745	0.259797	0.068404
C	-1.402531	1.481053	0.020691
C	-0.700524	2.67483	-0.02629
H	1.240148	3.613383	-0.063138
H	2.484548	1.473005	0.023486
H	-2.484832	1.472563	0.023196
H	-1.240805	3.613162	-0.063276
C	-1.40108	-1.003978	0.16492
C	1.401209	-1.003744	0.165068
O	-2.58749	-1.093348	-0.184696
O	-3.511463	-2.067664	0.019723

O	2.58772	-1.092885	-0.184275
O	3.511815	-2.067061	0.020275

Int12-M			
C	-3.147984	0.007109	0.050272
C	-2.153133	0.981153	0.024198
C	-0.807107	0.612949	-0.00036
C	-0.459022	-0.750103	-0.011254
C	-1.463108	-1.719	0.022423
C	-2.803125	-1.341577	0.057313
H	-4.189554	0.303313	0.07032
H	-2.410426	2.032827	0.039896
H	-1.185204	-2.765237	0.000157
H	-3.574935	-2.101111	0.077871
C	0.937619	-1.232672	-0.13347
C	0.192464	1.703211	0.085765
O	1.352496	-2.258901	0.460657
O	0.008345	2.834579	-0.434618
O	1.259059	1.638517	0.74201
O	1.801166	-0.714007	-0.882262

Int13-M			
C	2.658739	-1.447883	0.096351
C	1.301844	-1.743279	0.003259
C	0.35427	-0.721838	-0.039217
C	0.78568	0.615816	-0.012915
C	2.15046	0.906826	0.088719
C	3.083859	-0.12183	0.146605
H	3.382523	-2.253278	0.13406
H	0.95336	-2.767676	-0.028868
H	2.468562	1.941935	0.106215
H	4.139096	0.11176	0.222046
C	-0.126142	1.775677	-0.175874
C	-1.087456	-1.125749	-0.070262
O	-0.147567	2.735567	0.631913
O	-1.477357	-2.180507	-0.50942
O	-0.856563	1.94421	-1.182658
O	-1.86934	-0.193706	0.48458
C	-3.292188	-0.43722	0.44479
H	-3.743452	0.426228	0.925397
H	-3.624111	-0.523017	-0.589642
H	-3.52917	-1.354037	0.984226

TS7-M			
C	-1	-0.70771	-1.210487
C	0	-1.391128	-0.000565
C	0	-0.701378	1.216293
C	0	0.720152	1.223811
C	0	1.394262	-0.017549
C	-1	0.69152	-1.210487
H	0	-1.255724	-2.143901
H	0	-2.473341	0.015043
H	0	2.475745	-0.025435
H	0	1.232346	-2.149049
C	0	1.521292	2.40538
C	0	-1.510822	2.425119
O	0	2.798138	2.427981
O	0	-2.684252	2.544816
O	0	-1.183609	3.424649
O	0	1.162061	3.547075
C	0	1.19013	5.053974
H	0	0.249155	5.487489
H	0	1.214186	4.585401
H	0	2.100468	5.519526

Int14-M			
C	-0.67565	0.015928	0.11391
C	-1.498388	0.911898	-0.563067
C	-0.949918	1.94052	-1.326777
C	0.447922	2.046294	-1.431656
C	1.270073	1.147453	-0.743631
C	0.709765	0.137872	0.030887
H	-1.117114	-0.77203	0.712478
H	-2.5765	0.837848	-0.499283
H	2.345087	1.241211	-0.834735
H	1.352698	-0.553857	0.561642
C	1.128932	3.018303	-2.320344
C	-1.901782	2.911727	-1.954585
O	2.100906	3.715345	-1.933205
O	-3.021662	2.621116	-2.302604
O	0.877656	3.147113	-3.542351
C	1.027628	6.818689	-3.151657
H	0.815752	7.819656	-3.500819
H	1.34034	6.656459	-2.130149

H	1.012817	5.985258	-3.839216
O	-1.369314	4.133887	-2.030798
C	-2.167658	5.152486	-2.672298
H	-1.540792	6.040263	-2.677737
H	-2.411932	4.844252	-3.688727
H	-3.084681	5.316366	-2.1063

TS8-M			
C	-0.699075	0	0
C	-1.392754	-1.196048	-0.007343
C	-0.712101	-2.437902	0.010977
C	0.707072	-2.429464	0.070926
C	1.383934	-1.210469	0.029558
C	0.699075	0	0
H	-1.245154	0.936044	-0.018924
H	-2.474008	-1.197985	-0.068133
H	2.466354	-1.231306	0.043723
H	1.249023	0.933031	-0.017464
C	1.571348	-3.631765	0.234658
C	-1.52145	-3.610119	-0.177595
O	2.664282	-3.750019	-0.269554
O	-2.80961	-3.609342	0.05815
O	-1.173086	-4.753446	-0.635969
C	-1.374244	-6.273317	0.506484
H	-1.210022	-5.844534	1.484805
H	-2.384269	-6.561328	0.253827
H	-0.577363	-6.871091	0.088782
O	1.04776	-4.536726	1.084528
C	1.866258	-5.697907	1.32706
H	1.302568	-6.312482	2.024483
H	2.047939	-6.234558	0.395578
H	2.821025	-5.401348	1.761449

Pro-M			
C	-3.2031	-0.704963	0.066282
C	-1.986185	-1.366132	0.200446
C	-0.784741	-0.662313	0.113924
C	-0.80912	0.728871	-0.074642
C	-2.034438	1.382076	-0.222073
C	-3.227111	0.670262	-0.155012
H	-4.128606	-1.264793	0.127739
H	-1.953974	-2.436437	0.360863
H	-2.033411	2.453756	-0.376293
H	-4.17248	1.187761	-0.266521
C	0.416228	1.578997	-0.064725
C	0.475238	-1.466923	0.177982
O	0.551111	2.59862	-0.700909
O	0.693189	-2.324154	0.997208
O	1.303127	-1.170894	-0.842506
C	2.550208	-1.889838	-0.856717
H	3.075338	-1.541382	-1.742791
H	3.121532	-1.668808	0.046169
H	2.370293	-2.963517	-0.911993
O	1.341427	1.110803	0.794675
C	2.591915	1.815516	0.821914
H	3.197535	1.301814	1.564806
H	3.0672	1.774857	-0.159457
H	2.436901	2.857763	1.10352

References:

[1] H. Bader, *Ozone Sci. Eng.* **2008**, *4*, 169-176.

[2] E. J. de Melo, J. P. de Mesquita, M. C. Pereira, L. C. Duarte Cavalcante, E. d. Santos Filho, J. Domingos Fabris, J. D. Ardisson, L. C. Alves de Oliveira, *Hyperfine Interact* **2017**, *238*, 52.

[3] C. F. Chiou, B. J. Mariñas, J. Q. Adams, *Ozone Sci. Eng.* **1995**, *17*, 329-344.

[4] J. Zhou, Q. Wang, J. K. Cheng, W. Shen, R. N. Zare, X. Y. Sun, *J. Am. Chem. Soc.* **2025**, *147*, 10916-10924.

[5] Y. Meng, E. Gnanamani, R. N. Zare, *J. Am. Chem. Soc.* **2025**, *147*, 23399-23404.

[4] Frisch, M. J., Trucks, G. W., Schlegel, H. B. et al. GAUSSIAN 03, Gaussion, Inc., Pittsburgh, PA, **2009**.