Supporting Information

Mechanism and Kinetics for the Reaction of Methyl Peroxy Radical with O$_2$

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PES of H-Atom abstraction reaction

A product channel complex exists between CH_2OO and HO_2, PC1a, at 16.5 kcal/mol above the isolated reactants and requires 11.9 kcal/mol to break into the products CH_2OO and HO_2. An extensive reorientation along the surface is required to reach this configuration. In the presence of HO_2, CH_2OO in this complex further undergoes isomerization to a dioxirane complex with HO_2 with an energy barrier of 34.4 kcal/mol through TS2a. The product complex of dioxirane and HO_2 (PC2a) lies 5.8 kcal/mol below the isolated reactants. PC2a further isomerizes to methylenebis(oxy) isomer, PC3a by O-O bond cleavage through a transition state TS3a with energy barrier of 11.4 kcal/mol. PC3a lies just 1 kcal/mol below the TS3a and further undergoes unimolecular dissociation to several products. The methylenebis(oxy) isomer in PC3a results in the formation of formic acid, PC4a through an H-atom shift reaction passing via transition state TS4a with an activation energy of 2.4 kcal/mol with respect to the separated reactants. The product complex of formic acid and HO_2 is more stable by -95.6 kcal/mol.
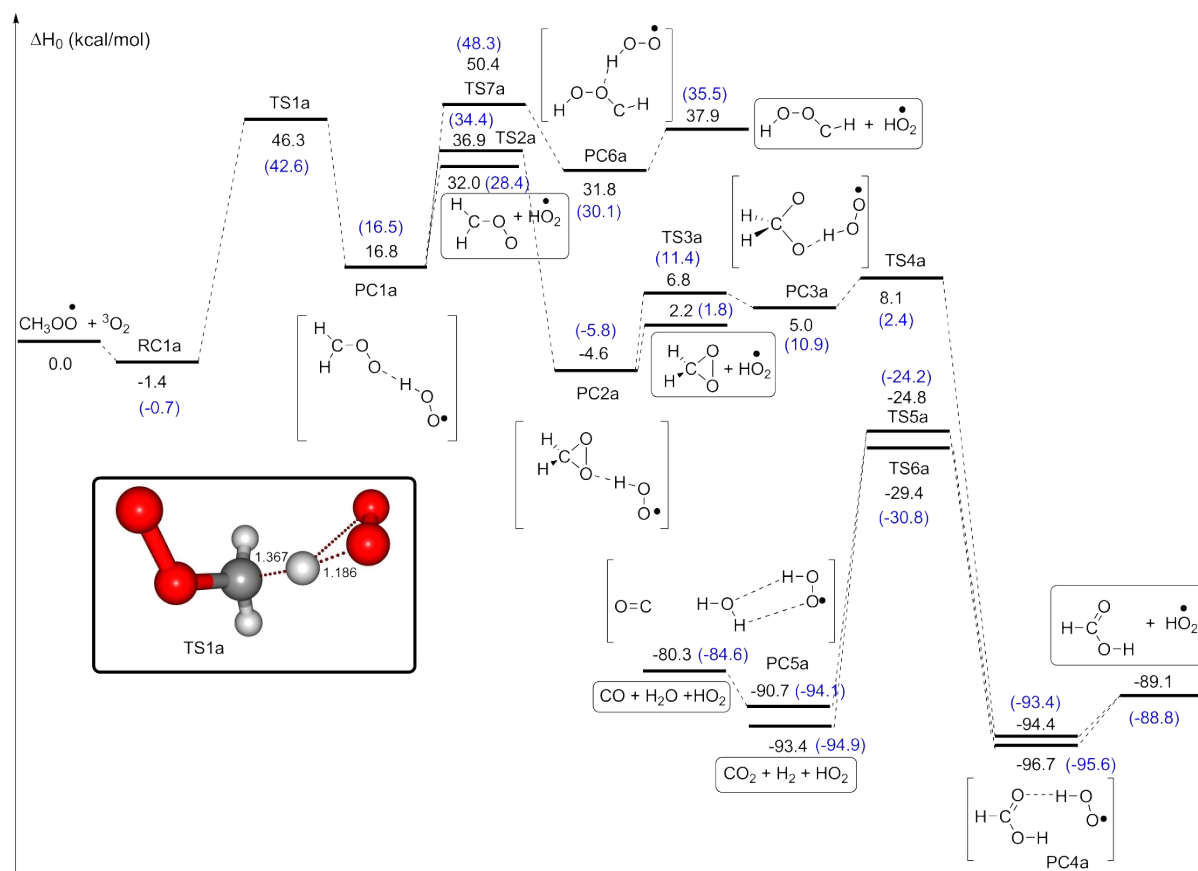
Figure S1: PES for the reaction between CH_3O_2 and $^3O_2$ through H-atom abstraction calculated at UM06-2X/cc-pVTZ level of theory. The values calculated at UCCSD(T)/cc-pVTZ//UM06-2X/cc-pVTZ level are in parenthesis. Energies, $\Delta H_0(0)$ are in kcal/mol.

The final products of CH_3O_2 oxidation through this pathway will be determined mainly from the decomposition routes of highly energetic formic acid product. The PES for formic acid dissociation was studied earlier[30,31] and $CO_2 + H_2$ and $CO + H_2O$ were identified as the main products. PC4a leads to two dissociation pathways, one forming $CO_2 + H_2 + HO_2$ as products and another forming $CO + H_2O + HO_2$ as products. These products are formed through transition states TS5a and TS6a with energy barriers of 71.4 and 64.8 kcal/mol with respect to PC4a. TS5a is a four-centred tight transition state in which the two H-atoms attached to C and O-atoms of formic acid migrate to form H_2. The reactions forming $CO_2 + H_2 + HO_2$ and $CO + H_2O + HO_2$ are highly exothermic by 92.7 and 82.2 kcal/mol, respectively, which is in good agreement with the ATcT[12] values of -94.1 and -84.3 kcal/mol. The $CH_2OO + HO_2$ (PC1a) complex can also undergo H-shift reaction resulting in $HCOOH + HO_2$ through transition state TS7a. The energy barrier required for this H-atom shift reaction is 48.3 kcal/mol, which is 13.9 kcal/mol higher than the energy barrier required for isomerization of CH_2OO to form dioxirane. This shows that the isomerization of CH_2OO is more favourable than the H-atom shift reaction.

The complexing of HO_2 with the various CH_2OO species involved in the reaction does not alter the energetics much. For instance, the key intermediates dioxirane and formic acid formed by isomerization of CH_2OO without complexing with HO_2 are exothermic by -24.5 and -118.6 kcal/mol, respectively calculated at UM06/6-311++G(d,p) level of theory with respect to CH_2OO in our previous study.[32] The formation of the same intermediates with HO_2 complexation are -22.5 and -113.1 kcal/mol at UM06-2X/cc-pVTZ level of theory calculated with respect to $CH_2OO + HO_2$ (PC1a) complex. The energy barrier also does not show any effect on HO_2 complexation. Irrespective of the methods used, there is no significant influence on the activation energy as well as enthalpy on HO_2 complexation with CH_2OO reactions. Taken together this result on the details of the surface and the high energy barrier associated with the initial step (TS1a), it may be concluded that the H-atom abstraction pathway is not a likely mechanism for significant $CH_3O_2 + O_2$ reaction.

Table S1: Cartesian coordinates(Å)of the structures of RC, PC and TS calculated at UM06-2X/cc-pVTZ level of theory

I. H-abstraction pathway

RC1a

6	1.117585000	-0.152398000	-0.129704000
1	1.734705000	0.074202000	0.737055000
1	1.382316000	-1.114374000	-0.559044000
1	1.192786000	0.642334000	-0.868503000
8	-0.249217000	-0.266829000	0.289559000
8	-0.675309000	0.845567000	0.804408000
8	1.669938000	2.825461000	1.393567000
8	1.307396000	3.222697000	0.333143000

TS1a

6	-0.510203000	0.841456000	0.278723000
1	-0.258433000	0.439364000	1.258154000
1	0.592503000	0.354271000	-0.367712000
1	-0.483818000	1.911461000	0.111140000
8	-1.612339000	0.299876000	-0.282062000
8	-1.912101000	-0.890625000	0.130340000
8	1.653813000	-0.106737000	-0.631488000
8	2.271997000	-0.271744000	0.448970000

PC1a

6	-1.208965000	0.970215000	0.169096000
1	-0.761973000	1.012495000	1.154418000
1	0.793904000	-0.908594000	0.033590000
1	-1.608503000	1.824793000	-0.364787000
8	-1.295754000	-0.112537000	-0.409503000
8	-0.749989000	-1.199598000	0.261686000
8	1.694747000	-0.466109000	-0.119167000
8	1.454791000	0.809496000	0.037259000

TS2a

6	0.920471000	0.892363000	-0.151304000
1	0.496186000	1.708319000	0.426409000
1	1.050725000	0.983371000	-1.223623000
8	1.512017000	-0.043430000	0.489772000
8	0.784843000	-0.966147000	-0.392147000
1	-0.665746000	-0.929435000	0.047863000
8	-1.613489000	-0.567320000	0.212569000
8	-1.483870000	0.687342000	-0.103047000

PC2a

6	1.374445000	0.659438000	-0.221723000
1	0.617486000	1.433987000	-0.256978000
1	2.387594000	0.902796000	-0.524878000
8	1.260009000	-0.251668000	0.809644000
8	0.945121000	-0.613408000	-0.574566000
1	-0.898575000	-0.863316000	-0.228074000
8	-1.800315000	-0.557713000	0.000836000
8	-1.698962000	0.744027000	0.056619000

TS3a

6	1.695193000	-0.011985000	0.130648000
1	2.071474000	-0.147779000	1.168340000
1	2.622309000	0.148480000	-0.459923000
8	1.121363000	-1.148377000	-0.278961000
8	0.982413000	1.133647000	0.120906000
1	-0.847254000	0.653323000	-0.263777000
8	-1.772775000	0.409634000	-0.458775000
8	-2.083212000	-0.467668000	0.463263000

PC3a

6	1.411515000	0.037179000	0.251177000
1	1.282510000	-0.070214000	1.347397000
1	2.504370000	0.178218000	0.114730000
8	1.065484000	-1.109912000	-0.350852000
8	0.784502000	1.177139000	-0.107588000
1	-0.919755000	0.437088000	-0.866740000
8	-1.762900000	0.077513000	-0.521709000
8	-1.504113000	-0.240761000	0.717343000

TS4a

6	1.328641000	0.044401000	0.276862000
1	1.726603000	-0.057843000	1.300259000
1	2.281310000	0.109047000	-0.417137000
8	1.102992000	-1.071786000	-0.383476000
8	0.773014000	1.176945000	-0.001326000
1	-0.938503000	0.628002000	-0.749002000
8	-1.768274000	0.175270000	-0.489359000
8	-1.487889000	-0.398630000	0.649750000

PC4a

6	1.084885000	-0.135771000	-0.000527000
1	0.550305000	-1.092569000	-0.001708000
1	2.699022000	-1.129311000	-0.000525000
8	2.413230000	-0.209755000	0.000353000
8	0.521462000	0.922088000	0.000192000
1	-1.222877000	0.834602000	-0.000430000
8	-2.121533000	0.423497000	-0.000203000
8	-1.880130000	-0.860592000	0.000387000

TS5a

6	1.245122000	-0.030053000	0.000095000
1	0.539734000	1.132837000	0.000319000
1	1.533343000	1.304633000	0.000422000
8	2.440117000	0.314644000	-0.000332000
8	0.522478000	-0.963009000	0.000380000
1	-1.350785000	-0.898133000	-0.001030000
8	-2.185035000	-0.384502000	-0.000252000
8	-1.801688000	0.862989000	0.000169000

TS6a

6	-2.135257000	0.327932000	0.017259000
1	0.119724000	0.217976000	0.986060000
1	-1.539867000	1.278561000	0.263796000
8	-0.267371000	0.605579000	0.186710000

8	-2.582246000	-0.696247000	-0.144317000
1	1.182780000	0.359739000	-0.613324000
8	2.128444000	0.044987000	-0.665340000
8	2.352286000	-0.432303000	0.530436000

PC5a

6	2.670873000	-0.039275000	0.029304000
1	-0.778274000	0.926957000	0.769566000
1	0.528893000	0.757344000	-0.031193000
8	-0.380333000	1.064944000	-0.098360000
8	3.722046000	-0.423487000	0.022654000
1	-1.641125000	0.062475000	-0.776031000
8	-2.466440000	-0.461098000	-0.616521000
8	-2.642114000	-0.369250000	0.674956000

TS7a

6	1.309628000	-0.899684000	-0.248682000
1	1.596328000	-1.847032000	0.219402000
1	0.929820000	0.088189000	-1.113548000
8	1.223775000	0.044443000	0.568692000
8	0.788675000	1.106627000	-0.315128000
8	-1.454621000	-0.797493000	-0.159975000
8	-1.743808000	0.425131000	0.196756000
1	-0.896083000	0.927273000	0.063481000

PC6a

6	1.696816000	0.890317000	0.171444000
1	2.190767000	1.495794000	-0.611120000
1	0.527489000	-0.561993000	1.185847000
8	1.328414000	-0.118973000	-0.471704000
8	0.625145000	-1.094420000	0.370915000
8	-1.569777000	0.733477000	0.408670000
8	-1.857771000	-0.200946000	-0.458911000
1	-1.107233000	-0.828812000	-0.395159000

II. O$_2$ addition pathways

TS1b

6	-1.609509000	0.636636000	0.094271000
1	-1.839598000	0.503851000	1.149706000
1	-1.003883000	1.526306000	-0.057808000
1	-2.528391000	0.699902000	-0.484503000
8	-0.956281000	-0.527925000	-0.410964000
8	0.083351000	-0.870567000	0.426552000
8	1.320678000	-0.319983000	-0.193758000
8	1.430868000	0.899740000	0.031542000

PC1b

6	1.451490000	0.355178000	0.099217000
1	0.885410000	1.153582000	0.574960000
1	2.356159000	0.144646000	0.665042000
1	1.688131000	0.605201000	-0.932484000
8	0.733404000	-0.891424000	0.155940000
8	-0.409320000	-0.779892000	-0.698259000
8	-1.450155000	-0.229594000	0.123631000

| 8 | -1.634934000 | 1.007889000 | -0.173360000 |

TS2b

6	1.149217000	0.779348000	0.227085000
1	-0.011411000	1.262261000	-0.227159000
1	0.984295000	0.871427000	1.301249000
1	2.020312000	1.275098000	-0.186133000
8	1.123863000	-0.493295000	-0.264062000
8	-0.164098000	-1.131208000	-0.083262000
8	-1.044193000	-0.217889000	0.465217000
8	-1.151635000	0.831783000	-0.399202000

PC2b

6	1.514992000	0.757422000	0.063866000
1	1.331762000	1.037895000	1.090795000
1	2.401749000	1.056795000	-0.473333000
1	-0.918593000	1.357077000	-0.536703000
8	1.113158000	-0.489201000	-0.312688000
8	-0.021203000	-0.868109000	0.441379000
8	-1.132878000	-0.480180000	-0.274939000
8	-1.447186000	0.837953000	0.088253000

TS3b

6	1.714268000	0.738970000	0.041653000
1	-2.069392000	0.843948000	0.694034000
1	1.391199000	1.139146000	0.995187000
1	2.745510000	0.798654000	-0.293822000
8	1.150681000	-0.453930000	-0.357000000
8	0.001536000	-0.757372000	0.509372000
8	-1.160007000	-0.545311000	-0.229330000
8	-1.536325000	0.854667000	-0.128706000

III. Concerted O$_2$-addition and H-atom abstraction pathways
RC1c

6	-1.531525000	0.981878000	0.134858000
1	-1.922270000	0.949634000	1.148993000
1	-0.527542000	1.399875000	0.124677000
1	-2.192666000	1.538942000	-0.522569000
8	-1.483774000	-0.351845000	-0.388251000
8	-0.732025000	-1.112078000	0.347727000
8	2.240951000	0.228235000	0.442516000
8	1.703803000	0.013223000	-0.597021000

TS1c

6	0.151012000	-0.748285400	0.328723100
1	0.068579900	-1.632220000	-0.111628300
1	0.197202400	-0.480244600	1.356038500
8	1.600852100	0.295837500	0.276246700
8	-0.916168900	-0.465156600	-0.287454900
8	-1.593193000	0.603472300	0.270019900
8	0.696060000	0.319778500	-0.599444700
1	1.307037800	-0.938336100	0.245487400

PC1c

| 6 | -0.072502000 | 0.943748000 | 0.277764000 |

1	0.893469000	-1.350303000	-0.008597000
1	-0.228132000	1.985634000	0.008341000
1	0.089045000	0.791295000	1.343564000
8	-1.327684000	0.301405000	-0.075874000
8	-1.224152000	-0.991673000	-0.036180000
8	0.972429000	0.462574000	-0.463845000
8	1.539485000	-0.658446000	0.199663000

TS2c

6	0.110943000	0.081752000	0.432877000
1	0.736704000	-1.057033000	0.270066000
1	-0.182462000	0.195896000	1.477343000
1	-2.704371000	0.337195000	-0.017598000
8	1.249915000	0.692939000	0.032108000
8	1.884190000	-0.607899000	-0.181173000
8	-0.902151000	0.282109000	-0.466445000
8	-2.046395000	-0.362970000	0.074626000

PC2c

6	0.836961000	-0.585016000	0.446937000
1	-1.858448000	0.223955000	-0.433394000
1	0.900632000	-1.225040000	1.329876000
1	0.550248000	0.909559000	-1.031957000
8	1.264304000	-0.810162000	-0.644329000
8	-2.064818000	-0.667466000	-0.099080000
8	0.202412000	0.549928000	0.778699000
8	0.021328000	1.377903000	-0.353558000

TS3c

6	0.697009000	-0.342299000	-0.012835000
1	-2.085904000	-0.529735000	0.291667000
1	-0.347181000	-0.890642000	-0.056669000
1	-0.877413000	1.843577000	-0.774580000
8	1.752479000	-0.862798000	-0.008246000
8	-1.657195000	-1.340071000	-0.028074000
8	0.578483000	1.013364000	0.038221000
8	-0.782712000	1.393328000	0.075173000

TS4c

6	-0.038418000	0.613433000	0.161665000
1	1.069709000	-0.647608000	1.268786000
1	-0.538028000	1.559207000	0.331526000
1	0.458584000	-0.198860000	1.659189000
8	-0.857798000	-0.425382000	-0.191534000
8	-2.112387000	-0.104713000	-0.013341000
8	1.166449000	0.613971000	-0.226861000
8	1.708765000	-0.633043000	-0.096951000

TS5c

6	-0.018622000	-0.647774000	0.212447000
1	0.270949000	-1.669015000	-0.050525000
1	0.074758000	-0.427697000	1.281167000
1	1.090426000	1.044957000	0.027646000
8	2.175423000	0.156054000	0.226514000
8	0.810974000	0.231892000	-0.529562000

8	-1.352566000	-0.460590000	-0.221091000
8	-1.799382000	0.689944000	0.207518000

TS6c

6	-0.230906000	0.843305000	0.271220000
1	-0.404799000	1.137608000	1.307566000
1	0.310722000	1.585424000	-0.307106000
8	-1.410012000	0.426251000	-0.369252000
8	-1.175790000	-0.904839000	0.025968000
8	0.397931000	-0.444044000	0.237195000
8	2.064382000	0.050182000	-0.221495000
1	2.467434000	-0.803261000	-0.007111000

Table S2: H$_{298}$ (Hartrees) of the reactive species calculated at various levels of theory

Species	CBS-QB3	G3B3	M06-2X/cc-pVTZ	UCCSD(T)/cc-pVTZ
CH$_3$OO	-189.954731	-190.088917	-190.157509	-189.8951244
O$_2$	-150.161303	-150.184576	-150.314423	-150.1210078
CO	-113.178703	-113.266664	-113.310376	-113.1466619
H$_2$O	-76.333711	-76.379947	-76.399905	-76.306806
HO$_2$	-150.737299	-150.826145	-150.885750	-150.6937276
CO$_2$	-188.368492	-188.500733	-188.576087	-188.3112222
OH	-75.646415	-75.693062	-75.718588	-75.6258244
H$_2$CO	-114.340363	-114.429933	-114.465762	-114.3027053
HCOOH	-189.523325	-189.656724	-189.727305	-189.4631695
H$_2$	-1.162774	-1.164167	-1.155393	-1.1588556

Table S3: Frequencies(cm⁻¹) of the stationary points calculated

RC1a		PC1a	TS2a	PC2a	TS3a	PC3a	TS4a
31.0301		63.4048	-699.534	62.4462	-54.0535	71.0549	-
54.4081		94.7676	103.1278	77.3522	46.3701	90.058	1161.8442
58.7136		187.29	146.529	147.0375	70.9394	148.5411	75.0113
75.567		259.3419	185.2682	176.5114	111.8913	163.1459	104.1687
116.9052		325.3637	319.3648	219.4192	205.8098	216.9196	120.4772
163.4906		518.2874	401.2648	479.7473	377.4302	389.8924	171.2608
515.898		689.5996	828.5349	916.2491	597.723	606.3824	222.7391
984.4969		816.5549	905.6426	937.5574	607.1657	610.4204	413.0036
1149.6167		872.3585	998.3916	1062.4542	918.5521	939.5098	480.8587
1204.6709		1115.9296	1140.3181	1196.2281	949.542	964.395	668.8585
1293.4755		1254.4096	1218.0314	1281.8043	1143.586	1134.9768	977.3264
1458.684		1306.2227	1322.2676	1283.4178	1223.5638	1235.3018	1143.721
1485.6396		1452.3891	1419.6999	1365.7514	1270.0388	1282.279	1280.3593
1495.992		1648.2067	1573.2137	1518.286	1289.7375	1296.8292	1290.0749
1757.6608		1694.1795	1623.7945	1546.4871	1525.4992	1517.7324	1369.4691
3083.3164		2863.2887	2680.2022	3124.0747	2890.7186	2908.0238	1518.8705
3174.1125		3144.7141	3119.6642	3239.5308	2920.9837	2941.5978	2439.4478
3190.3378		3290.4967	3252.0343	3575.634	3620.6423	3589.9073	2989.2913
							3564.6204

PC4a	TS5a	TS6a	PC5a	TS7a	PC6a		PC1b
64.523	-2218.7946	-1641.6559	16.2025	-1736.9334	33.3739		57.5167
83.4688	50.9937	24.663	37.6294	82.9029	68.6268		160.3332
128.0962	90.7548	62.1539	88.927	92.0816	133.147		189.5632
176.6748	120.3683	95.6775	106.7117	200.6004	162.0996		348.0588
229.1677	160.5857	178.5152	108.0268	206.5939	246.297		386.0537
545.23	215.2128	290.6196	183.8298	278.689	476.9349		502.9047
639.2846	448.9841	331.419	287.8667	726.1316	554.9009		739.1169
697.0035	603.426	466.5588	308.2647	783.8744	577.5664		999.5546
1086.5906	763.0331	698.7282	415.519	807.8307	707.986		1106.0665
1176.5496	1026.4205	721.6318	526.1583	941.9847	877.4625		1184.5758
1291.5101	1030.8812	750.3844	715.7445	1180.2717	1276.3252		1229.5056
1307.4421	1288.3265	1058.5823	1290.5533	1288.0923	1295.9503		1401.9088
1435.7875	1413.6674	1292.4952	1579.7922	1293.9857	1385.7749		1461.8599
1558.5106	1505.4856	1610.1439	1626.854	1561.2888	1473.9175		1483.9404
1866.4056	1908.4331	2045.1267	2299.3094	1575.3251	1512.7019		1511.4307
3091.1014	2141.8816	2688.8125	3358.5522	2126.4909	2983.5075		3069.9466
3384.1702	2205.6952	3187.554	3814.5657	3102.047	3561.2695		3152.7585
3870.4966	3575.7782	3785.8542	3905.3367	3263.8404	3641.4329		3177.2985

TS2b	PC2b	TS3b			PC1c	TS2c	PC2c
-1973.7375	91.4215	-209.1425			60.2044	-1802.1438	-96.1195
152.6529	180.2072	100.5357			136.6876	98.358	69.7167
392.5624	265.7655	155.2318			252.3333	182.648	137.7923
509.2484	387.7534	373.5406			339.246	211.8896	254.2314
563.3733	455.7658	441.6479			422.5678	346.8591	329.5879
634.1992	524.8791	526.7428			611.538	526.3668	359.1653
738.5482	656.6591	532.2423			1024.935	738.7254	422.0715
837.316	732.3988	656.5829			1048.1478	932.1743	528.7239
916.0173	837.4119	844.7649			1142.7601	1023.562	869.8247
1039.1571	949.0706	932.4026			1174.1744	1053.6851	965.2751
1095.1235	1012.1833	1009.0553			1231.6639	1167.1655	1030.7197
1152.3509	1170.9849	1162.8627			1289.513	1176.7999	1202.3381
1218.5772	1219.466	1213.0681			1414.099	1217.4419	1376.4169
1281.1291	1444.3429	1426.7064			1430.2526	1358.2831	1505.6206
1447.6202	1446.6991	1445.303			1520.1582	1440.3936	1853.0064
1715.248	3156.2448	3178.135			3086.2809	2019.5173	3134.2017
3077.5462	3300.1444	3328.3991			3159.0366	3107.13	3595.2563
3217.2006	3764.6853	3795.6841			3828.4929	3837.6871	3734.5037

TS3c	TS4c	TS5c	TS6c				
-910.4754	-983.3287	-1171.0708	-1220.6497				
112.7525	99.7515	73.8723	117.5899				
158.0489	253.2795	142.2217	204.8278				
182.3726	457.9741	298.5923	244.434				
242.457	543.9513	386.3687	284.6332				
362.2131	693.4066	600.6625	434.5333				
412.6542	734.2064	816.2229	761.4068				
590.904	813.1592	987.4756	900.8754				
725.0502	981.0392	1026.6557	973.0044				
893.4698	1048.979	1089.7795	1042.6376				
1019.9107	1131.4181	1199.6632	1128.0413				
1064.3223	1144.3514	1250.8938	1155.2695				
1139.9059	1258.6466	1294.111	1202.3972				
1437.288	1302.2027	1387.577	1383.4492				
1462.7617	1397.9485	1477.0044	1533.8721				
1947.3109	1530.1326	3140.0001	3079.3675				
3788.9067	2733.6864	3181.0348	3184.5485				
3821.3648	3228.1654	3238.9978	3823.7418				

Table S4: $H_0(0)$ [Hartrees] of the stationary points involved in the studied reaction calculated at UM06-2X/cc-pVTZ and UCCSD(T)//UM06-2X/cc-pVTZ level of theories.

Stationary points	UM06-2X/cc-pVTZ	UCCSD(T)//UM06-2X/cc-pVTZ
H-atom abstraction		
RC1a	-340.481317	-340.0244205
TS1a	-340.405257	-339.9552524
PC1a	-340.452254	-339.9969768
TS2a	-340.420213	-339.9683894
PC2a	-340.486824	-340.0305377
TS3a	-340.468176	-340.0050478
PC3a	-340.471030	-340.0056978
TS4a	-340.466106	-340.0193993
PC4a	-340.629470	-340.1720749
TS5a	-340.518576	-340.0617314
PC5a	-340.623557	-340.1732302
TS6a	-340.525823	-340.072417
TS7a	-340.398702	-339.946232
PC6a	-340.428346	-339.9751751
O$_2$ addition		
TS1b	-340.440689	-339.9883501
PC1b	-340.442589	-339.9927961
TS2b	-340.389000	-339.9272567
PC2b	-340.418285	-339.9632495
TS3b	-340.383807	-339.9601229
Concerted H-atom abstraction and O$_2$ addition		
RC1c	-340.481317	-340.0244205
TS1c	-340.469144	-340.00170793
PC1c	-340.514860	-340.0552219
TS2c	-340.441771	-339.9849644
PC2c	-340.581895	-340.1261627
TS3c	-340.570145	-340.1138163
TS4c	-340.423270	-339.9367327
TS5c	-340.423376	-339.9676583
TS6c	-340.405742	-339.9607891