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Supporting Information

Atmospheric Oxidation Mechanism and Kinetics of 1, 3, 5-Trimethylbenzene Initiated by OH radical- A Theoretical Study

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Table S1: The relative energy (ΔE in kcal/mol), enthalpy (ΔH in kcal/mol) and Gibbs free energy (ΔG in kcal/mol) for the initial reaction of 1,3,5-TMB with OH radical calculated at M06-2X, w-B97XD, MPW1K, UCCSD(T) with 6-311++G(d,p) basis set and from CBS-QB3, G3B3 and ROCBS-QB3 methods. T1-diagonestic value (T1) for the reactive species calculated at RCCSD(T)/6-311++(d,p) method.

Species	M06-2X			w-B97XD			MPW1K			UCCSD(T)			CBS-QB3			G3B3			ROCBS-QB3			RCCSD(T)			
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	T1
R	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-
RC1	-3.3	-5.7	-7.6	-2.5	-4.1	-6.3	-3.5	-5.3	-6.8	-4.1	-6.8	-8.5	-4.8	-7.3	-9.8	-5.1	-8.0	-9.6	-4.1	-6.9	-9.6	-3.8	-6.2	-8.1	0.01
TS1	4.7	6.3	8.9	9.3	11.6	13.4	7.2	8.8	9.3	6.9	7.2	8.5	7.3	8.4	9.9	6.8	7.95	9.2	7.6	9.3	10.0	6.1	7.8	8.4	0.02
IC1	-10.6	-12.4	-14.7	-8.4	-10.3	-12.6	-10.8	-11.4	-12.5	-10.5	-13.5	-14.9	-10.3	-12.2	-15.3	-12.7	-14.2	-16.8	-9.3	-11.2	-14.8	-9.8	-12.3	-13.7	0.02
I1+H_2O	-7.3	-9.6	-12.5	-6.6	-8.5	-9.4	-7.1	-8.6	-10.7	-8.5	-10.7	-13.0	-9.0	-11.8	-13.8	-10	-12.7	-14.5	-8.2	-10.8	-13.3	-8.2	-10.1	-12.1	0.01
TS2	7.5	9.8	11.4	5.6	7.1	8.5	8.1	9.4	10.8	6.2	7.5	9.1	5.1	6.5	8.3	5.4	7.1	8.6	5.5	7.1	9.2	5.9	7.1	9.8	0.01
IC2	-8.4	-10.6	-12.6	-7.1	-8.5	-9.7	-6.2	-7.7	-9.1	-8.3	-9.9	-10.2	-9.8	-11.4	-13.1	-12.5	-14.1	-15.7	-8.5	-10.3	-12.9	-7.6	-8.8	-9.5	0.02
I2+H_2O	-5.7	-7.6	-9.3	-4.3	-6.5	-7.8	-5.8	-8.0	-10.5	-7.3	-9.1	-10.7	-8.4	-10.2	-12.4	-9.1	-10.8	-12.9	-7.6	-9.6	-12.1	-6.9	-8.2	-11.3	0.01
TS3	3.1	5.4	7.2	4.6	6.8	8.0	6.5	5.2	7.4	4.0	4.4	5.6	4.6	5.5	6.5	2.3	3.8	5.9	6.3	7.4	6.7	4.8	5.1	6.2	0.02
I3	-12	-14.3	-16.6	-10.7	-12.4	-14.6	-11.3	-12.6	-14.4	-15.4	-17.5	-18.2	-14.7	-16.2	-18.1	-17	-17.4	-19.2	-13.8	-15.1	-17.6	-14.6	-16.3	-17.4	0.02
TS4	1.6	3.4	5.1	2.8	3.9	5.1	3.0	4.3	5.2	0.6	2.2	3.9	1.9	2.5	3.3	1.1	2.2	3.1	3.1	3.5	4.1	0.4	2.5	4.4	0.01
I4	-14.1	-17.5	-19.0	-16.4	-17.4	-18.8	-15.7	-16.1	-17.4	-18.8	-19.2	-21.2	-17.2	-20.0	-22.4	-17.1	-19.8	-21.8	-16.4	-18.6	-22.1	-17.5	-18.7	-18.8	0.01

Table S2: The relative energy (ΔE in kcal/mol), enthalpy (ΔH in kcal/mol) and Gibbs free energy (ΔG in kcal/mol) for the reaction of I1 with O_2 and I5 with HO_2 and NO radicals calculated at M06-2X, w-B97XD, MPW1K, UCCSD(T) and RCCSD(T) with 6-311++G(d,p) basis set and CBS-QB3 and G3B3 and ROCBS-QB3 methods. T1-diagonestic value (T1) for the reactive species calculated at RCCSD(T)/6-311++(d,p) method.

Species	M06-2X			w-B97XD			MPW1K			UCCSD(T)			CBS-QB3			G3B3			ROCBS-QB3			RCCSD(T)			
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	T1
I1+O_2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.01
I5	-31.5	-33.1	-34.4	-30.3	-32.4	-34.9	-32.6	-33.6	-36.6	-32.6	-34.1	-36.7	-33.9	-35.7	-37.4	-34.5	-35.1	-36.6	-33.6	-35.2	-37.3	-31.8	-33.6	-35.7	0.02
I5+HO_2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-
RC2	-11.5	-13.3	-15.7	-10.4	-11.8	-13.1	-9.8	-11.2	-12.4	-13.6	-15.7	-17.5	-14.0	-15.9	-17.2	-14.8	-16.1	-18.2	-12.7	-15.1	-17.1	-12.6	-14.9	-16.6	0.01
TS5	2.4	4.5	6.9	3.4	6.1	7.5	4.10	6.8	8.1	1.8	3.2	5.4	2.9	5.1	8.3	3.0	5.8	8.9	3.1	5.8	8.4	2.3	3.8	5.9	0.01
PC1	-41.8	-44.5	-47.3	-40.5	-41.8	-43.4	-41.8	-42.7	-43.0	-42.1	-44.1	-46.2	-44.5	-46.3	-47.9	-43.4	-46.2	-48.8	-43.6	-45.6	-47.9	-41.9	-43.6	-45.2	0.02
P1+O_2	-29.2	-31.6	-34.8	-28.5	-29.7	-31.1	-29.3	-30.5	31.8	-30.4	-32.7	-35.0	-31.5	-33.5	-35.6	-32.0	-34.5	-37.1	-31.1	-33.1	-35.6	-30.1	-31.9	-34.4	0.03
I5+NO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.02
I6	-36.4	-37.6	-39.8	-34.7	-36.2	-38.6	-35.4	-36.7	-38.8	-35.7	-36.2	-37.5	-37.6	-38.4	-41.4	-38.6	-39.7	-41.8	-36.8	-38.4	-41.3	-34.7	-35.4	-36.8	0.02
TS6	5.8	8.5	9.1	6.5	7.4	8.2	5.1	8.45	9.2	4.3	7.5	8.5	3.8	6.6	7.2	4.4	7.2	8.3	4.1	7.1	7.8	4.6	8.3	9.3	0.01
I7+NO_2	-39.4	-38.7	-37.6	-37.5	-38.2	-39.7	-40.2	-37.6	-38.5	-38.6	-39.4	-40.6	-40.6	-39.7	-40.4	-41.2	-40.2	-39.6	-39.8	-39.2	-40.0	-37.5	-38.8	-39.5	0.01
I7+O_2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-
RC3	-9.4	-11.7	-13.6	-8.3	-10.5	-12.4	-9.8	-11.0	-13.7	-11.6	-13.2	-15.2	-12.1	-14.3	-16.7	-12.5	-14.8	-16.3	-11.4	-14.1	-16.5	-11.2	-12.6	-14.2	0.03
TS7	4.4	6.8	8.6	5.1	6.4	7.7	5.7	6.8	7.1	4.7	6.0	7.3	4.4	5.4	6.4	4.1	5.8	6.4	4.9	5.5	6.6	5.2	5.50	7.8	0.02
PC2	-35.7	-38.5	-40.3	-36.3	-37.8	-38.7	-36.9	-37.5	-39.9	-36.6	-39.2	-41.5	-35.5	-40.8	-42.9	-36.7	-41.5	-42.9	-34.7	-40.6	-42.5	-35.4	-38.4	-40.7	0.03
P2+HO_2	-28.9	-30.6	-32.5	-27.1	-29.5	-31.6	-28.4	-29.8	-31.5	-30.4	-32.7	-33.8	-31.0	-33.1	-35.3	-31.6	-33.4	-35.1	-31	-33.1	-35.3	-29.9	-32.1	-34.8	0.02

Table S3: The relative energy (ΔE in kcal/mol), relative enthalpy (ΔH in kcal/mol) and Gibbs free energy (ΔG in kcal/mol) for the reaction of I4 with O_2 and subsequent reactions calculated at M06-2X, w-B97XD, MPW1K, RCCSD(T) and UCCSD(T) with 6-311++G(d,p) basis set and CBS-QB3, G3B3 and ROCBS-QB3 methods. T1-diagonestic value (T1) for the reactive species calculated at RCCSD(T)/6-311++(d,p) method.

Species	M06-2X			w-B97XD			MPW1K			UCCSD(T)			CBS-QB3			G3B3			ROCBS-QB3			RCCSD(T)			
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	T1
$I4+O_2$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.01
RC4	-2.3	-4.8	-7.2	-2.0	-3.4	-5.6	-3.0	-4.7	-6.1	-3.5	-5.8	-8.14	-4.7	-6.1	-9.1	-5.1	-7.8	-10.0	-4.5	-5.6	-8.6	-2.9	-4.6	-7.5	0.01
TS8	1.8	3.1	5.4	2.3	4.3	6.9	2.7	5.1	7.3	1.3	2.5	3.6	1.0	2.6	3.5	0.5	2.0	3.2	1.4	3.2	4.1	1.5	2.8	4.2	0.03
PC3	-43.2	-46.4	-49.8	-42.6	-44.7	-47.2	-43.1	-45.2	-48.4	-44.6	-47.8	-50.9	-45.1	-48.6	-51.5	-46.0	-49.3	-52.2	-39.8	-47.6	-50.7	-43.4	-47.1	-50.1	0.03
$P3+HO_2$	-32.2	-34.8	-37.5	-31.1	-33.2	-36.8	-34.7	-36.4	-37.	-37.2	-38.5	-39.1	-37.5	-38.6	-39.8	-35.1	-37.1	-40.3	-37.1	-37.8	-39.3	-36.3	-37.9	-38.3	0.04
I8	-52.6	-54.2	-42.9	-52.5	-53.3	-54.9	-51.3	-52.3	-54.8	-53.5	-56.3	-57.0	-53.3	-55.7	-57.4	-55.2	-56.9	-58.2	-52.8	-55.1	-56.6	-52.8	-55.4	-56.4	0.02
TS9	9.7	11.4	12.	10.3	11.6	12.8	9.1	10.4	11.3	8.7	9.66	10.1	8.7	9.6	10.4	8.8	10.1	11.3	9.2	10.1	10.8	8.6	9.8	10.7	0.02
I9	-37.3	-40.1	-41.5	-36.7	-38.9	-39.5	-36.9	-38.4	-39.7	-35.2	-38.3	-40.6	-38.3	-42.5	-43.5	-39.9	-42.8	-44.3	-37.9	-41.7	-43.2	-34.1	-37.2	-39.2	0.02
TS10	14.6	15.1	16.5	16.0	17.5	18.4	15.8	16.6	18.3	13.3	14.3	15.9	12.1	13.4	14.6	15.4	16.8	14.7	12.6	13.8	15.1	13.7	14.7	16.4	0.02
I10	-25.7	-27.2	-29.8	-23.5	-25.0	-26.9	-24.4	-25.8	-27.2	-28.3	-27.5	-28.3	-23.6	-24.3	-28.4	-30.4	-31.2	-30.8	-23.2	-23.6	-27.7	-26.9	-26.4	-27.4	0.02
TS11	16.8	18.4	19.1	17.6	18.9	20.3	16.3	17.7	19.1	14.5	16.8	18.	15.6	16.8	17.6	14.0	15.3	17.0	16.2	17.4	17.9	15.2	17.1	19.2	0.02
I11	-23.6	-26.7	-27.6	-22.5	-23.1	-25.0	-24.1	-25.2	-26.3	-26.9	-26.4	-27.9	-27.1	-28	-30.2	-28.2	-29.5	-30.5	-26.5	-27.6	-29.8	-25.6	-25.2	-27.4	0.01
$I9+O_2$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.02
TS12	14.7	16.6	17.5	15.3	16.5	17.8	14.5	15.6	16.0	12.3	13.9	15.4	14	15	17.9	13.2	14.4	13	13.7	15.5	18.4	12.8	14.6	16.3	0.03
I12	-29.9	-31.2	-33.9	-28.1	-30.1	-31.5	-30.1	-32.3	-33.7	-31.3	-33.5	-35.1	-31.2	-33.8	-34.8	-32.4	-34.3	-36	-30.4	-33.2	-34.3	-30.7	-32.5	-33.8	0.03

Table S4: The relative energy (ΔE in kcal/mol) relative enthalpy (ΔH in kcal/mol) and Gibbs free energy (ΔG in kcal/mol) for the reaction of I12 with HO_2, and NO radicals calculated at M06-2X, w-B97XD, MPW1K, UCCSD(T) and RCCSD(T) with 6-311++G(d,p) basis set and CBS-QB3, G3B3 and ROCBS-QB3 methods. T1-diagonestic value (T1) for the reactive species calculated at RCCSD(T)/6-311++(d,p) method.

Species	M06-2X			w-B97XD			MPW1K			UCCSD(T)			CBS-QB3			G3B3			ROCBS-QB3			RCCSD(T)			
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	T1
I12+HO_2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-
RC5	-6.1	-8.5	-11.4	-5.4	-7.4	-10.6	-6.0	-9.0	-11.8	-7.3	-10.2	-13.8	-8.4	-10.0	-12.9	-8.9	-11.5	-13.7	-7.9	-9.8	-11.8	-6.5	-9.5	-12.6	0.02
TS13	1.8	4.3	6.6	2.1	5.4	7.8	2.9	4.9	7.6	1.3	2.9	5.8	0.9	3	4.2	0.5	2.1	3.6	1.2	3.1	5.2	2.1	3.7	6.6	0.02
PC4	-42.0	-44.2	-47.4	-41.8	-43.1	-46.1	-42.3	-45.2	-48.0	-44.5	-47.8	-49.2	-45.3	-48.5	-50.6	-44.1	-46.2	-49.2	-44.1	-47.9	-49.7	-39.7	-46.4	-48.5	0.03
P4+O_2	-28.2	-30.8	-33.5	-27.0	-29.5	-32.3	-28.1	-30.4	-32.8	-29.9	-31.9	-34.1	-30.1	-32.6	-35.7	-31.2	-33.6	-36.2	-29.8	-32.3	-34.5	-29.1	-31.3	-33.4	0.03
I12+NO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.02
I13	-33.8	-34.6	-36.9	-34.3	-35.5	-37.2	-33.7	-34.1	-35.6	-34.4	-36.6	-38.8	-36.4	-37.6	-39.5	-36.8	-37.9	-39.8	-35.1	-37.4	-39.2	-33.8	-37.5	-37.9	0.02
TS14	7.7	9.6	11.0	10.3	12.7	13.8	10.5	11.3	13.4	8.5	9.8	11.5	8.1	10.2	11.5	8.5	9.9	10.7	8.5	10.5	11.3	9.6	9.1	12.4	0.02
I14+NO_2	-36	-37	-38.6	-31.9	-34.1	-36.7	-32.9	-34.5	-37.7	-34.4	-36.0	-38.1	-35.5	-39.1	-41.5	-35.7	-37.3	-40.7	-34.1	-39.1	-41.4	-33.6	-35.5	-37.6	0.01
I14+O_2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.02
RC6	-7.8	-10.8	-13.5	-8.5	-9.9	-12.0	-6.53	-8.5	-11.9	-9.9	-12.3	-14.7	-10.4	-13	-15.2	-9.9	-13.6	-16	-8.6	-13.4	-15.5	-9.1	-11.6	-13.3	0.02
TS15	2.1	3.6	6.2	3.8	5.1	6.3	3.7	5.4	6.8	1.7	2.6	4.4	1.3	2.3	3.6	1.9	2.8	4.5	1.9	2.57	4.4	2.2	3.1	5.4	0.02
PC5	-32.5	-35.3	-38.0	-31.0	-33.9	-36.7	-33.2	-35.8	-39.1	-34.1	-37.5	-40	-35.1	-37.9	-40.5	-35.2	-38.0	-41.1	-34.7	-37.1	-39.9	-33.5	-36.8	-39.3	0.03
P5+HO_2	-26.9	-29.4	-31.6	-25.1	-27.2	-29.8	-27.0	-30.6	-31.9	-28.5	-30.8	-32.3	-29.3	-32	-31.3	-28.6	-31.4	-34.6	-29.2	-32.1	-33.3	-27.7	-31.3	-31.5	0.02
I14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.03
TS16	13.5	15.6	16.3	14.6	15.2	16.6	14.0	15.4	16.7	11.2	13.7	15.2	11.6	13.8	14.4	12.7	14.2	16.5	12.3	14.3	14.6	10.4	12.9	15.8	0.01
I15	-23.4	-25.4	-27.2	-22.7	-24.6	-26.8	-24.2	-25.3	-26.4	-25.3	-27.4	-28.8	-26.5	-27.2	-28.5	-27.5	-28.4	-29.6	-26.1	-26.3	-28.2	-24.8	-26.8	-27.2	0.02
TS17	15	17.8	19	15.6	17.1	18.6	16.2	17.5	18.4	13.6	15.9	17.1	12.9	14.6	16.3	13.6	15.3	18	13.8	15.3	16.5	14.2	16.5	17.6	0.02
P6+I16	-18.4	-19.3	-20.5	-16.8	-18.4	-19.3	-17.4	-18.9	-20.5	-19.3	-20.1	-22.5	-21.8	-23.2	-24.4	-20.6	-21.6	-23.8	-21.2	-22.1	-24	-18.7	-19.5	-21.7	0.03
I16+O_2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-
RC7	-4.3	-6.6	-8.8	-3.5	-5.1	-7.4	-4.0	-6.0	-7.2	-5.1	-7.9	-10.0	-6.3	-8.9	-10.9	-7	-9.1	-11.5	-5.7	-8.2	-10.1	-4.5	-7.2	-9.1	0.02
TS18	2.5	4.1	6.7	3.5	5.5	7.7	3.0	5.2	8.4	1.7	2.3	4.6	1.2	2.4	3.9	1.1	2.7	4.1	1.7	3.4	4.8	2.3	2.8	5.3	0.02
PC6	-49.3	-51.8	-54.1	-48.5	-50.8	-53.3	-47.9	-49.5	-52.9	-50.6	-52.2	-55.5	-52.0	-54.3	-56.5	-52.8	-54.6	-57.3	-51.1	-53.8	-55.4	-49.6	-51.6	-54.8	0.03
P7+HO_2	-41.6	-43.5	-45.7	-40.1	-42.2	-44.6	-39.8	-41.7	-43.7	-42.9	-45.1	-47.2	-43.6	-46.0	-47.6	-44.2	-46.1	-48.2	-42.7	-45.5	-46.8	-42.1	-44.3	-46.5	0.03

Table S5: The TST, TST (SCT), CVT and CVT (SCT) rate constants (in $cm^3molecule^{-1}s^{-1}$) for the initial H-abstraction reaction (I1 and I2) and OH addition (I3 and I4) reactions of 135-TMB with OH radical.

Temp (in K)	I1				I2				I3				I4			
	TST ($x10^{-15}$)	CVT ($x10^{-15}$)	TST (SCT) ($x10^{-13}$)	CVT (SCT) ($x10^{-13}$)	TST ($x10^{-16}$)	CVT ($x10^{-16}$)	TST (SCT) ($x10^{-14}$)	CVT ($x10^{-14}$)	TST ($x10^{-14}$)	CVT ($x10^{-14}$)	TST (SCT) ($x10^{-13}$)	CVT (SCT) ($x10^{-13}$)	TST ($x10^{-13}$)	CVT ($x10^{-13}$)	TST (SCT) ($x10^{-12}$)	CVT (SCT) ($x10^{-12}$)
250	2.2	1.8	2.7	2.3	0.06	0.05	1.3	1.0	0.3	0.3	6.5	5.8	0.7	0.7	7.4	6.9
258	2.7	2.4	3.4	3.1	0.08	0.07	2.4	1.9	0.6	0.4	7.2	6.4	0.9	0.8	8.9	7.5
268	3.3	3.0	4.2	3.8	0.1	0.09	3.7	3.0	0.8	0.7	8.0	7.2	1.3	1.0	10.0	8.7
278	3.9	3.7	4.9	4.5	0.4	0.2	4.9	4.2	0.9	0.8	8.7	8.1	2.3	2.1	11.6	9.6
288	4.5	4.2	5.7	5.2	0.5	0.4	5.8	5.3	1.2	1.1	9.4	8.9	3.1	2.7	12.6	10.4
298	5.2	4.9	6.5	6.0	0.7	0.6	7.0	6.5	2.1	1.8	10.3	9.6	3.8	3.5	13.9	11.8
308	6.3	5.7	7.3	6.9	0.9	0.8	8.4	7.9	3.0	2.6	11.0	10.4	4.5	4.3	15.1	13.0
318	7.0	6.6	8.0	7.7	1.8	1.4	9.4	8.3	3.5	3.2	11.9	11.1	5.2	4.9	16.3	14.7
328	7.8	7.3	8.8	8.4	2.6	2.2	10.2	9.8	4.8	4.3	12.7	12.0	6.2	5.7	17.9	16.1
338	8.6	8.0	9.3	9	3.4	2.9	11.4	10.7	5.8	5.3	13.5	12.9	7.1	6.6	19.03	17.5
348	9.2	8.8	10.3	9.5	4.6	4.0	12.5	11.3	6.5	6.1	14.2	13.4	7.9	7.4	20.3	19.2
350	9.3	9.0	10.5	10.5	4.9	4.4	12.8	12.8	7.0	6.4	14.8	14.7	8.1	7.9	20.6	19.7