

Table S1: Changes in the reactions of C₀-C₆ species.

Reactions	A	n	E _a	References
C₀-C₂ reaction base				
HO ₂ +CO=CO ₂ +OH	1.6×10 ⁵	2.2	17.9	[38]
H ₂ O ₂ (+M) =2OH (+M)	2.0×10 ¹²	0.9	48.7	[19]
HE/0.44/ AR/0.68/ O ₂ /0.79/ N ₂ /1.00/ CO ₂ /1.06/ H ₂ O/5.1/ H ₂ O ₂ /5.2/ LOW /3.65×10 ²⁴ -2.3 4.8749×10 ⁴ / TROE /0.43 1 1.0×10 ⁸ /				
HCHO+OH=CHO+H ₂ O	7.8×10 ⁷	1.6	-1.06	[39]
C ₂ H+OH=C ₂ H ₂ +O	1.8×10 ¹³	0.0	0.0	[40]
C₃-C₅ reaction base				
C ₂ H ₃ CHO+O ₂ =CH ₂ CHCO+OOH	3.0×10 ¹³	0.0	38.5	estimated ^a
C ₃ H ₆ +OH=HCHO+C ₂ H ₅	1.5×10 ¹²	0.0	-0.9	[41]
C ₃ H ₆ +OH=CH ₃ +CH ₃ CHO	1.5×10 ¹²	0.0	-0.9	[41]
C ₃ H ₇ +O ₂ =HO ₂ +C ₃ H ₆	3.7×10 ¹⁶	-1.63	3.42	[42]
C ₄ H ₄ +C ₂ H ₂ =C ₆ H ₅ +H	1.0×10 ⁹	0.0	30.0	[43]
C ₄ H ₅ +O ₂ =CHO+C ₂ H ₃ CHO	5.7×10 ²⁸	-5.31	6.5	estimated ^b
C ₄ H ₅ +O ₂ =C ₂ H ₄ +CO+CHO	1.1×10 ²⁹	-5.31	6.5	estimated ^b
C ₄ H ₅ +O ₂ =C ₄ H ₄ +HO ₂	5.2×10 ¹⁵	-1.26	3.31	estimated ^b
C ₄ H ₆ -1=C ₃ H ₃ +CH ₃	3.0×10 ¹⁵	0.0	75.8	[44]
C ₅ H ₄ O+H=C ₅ H ₃ O+H ₂	8.1×10 ⁷	2.03	15.9	estimated ^c
C ₅ H ₄ OH+HO ₂ =>OH+OH+C ₅ H ₄ O	3.0×10 ¹²	0.0	0	estimated ^d
C ₅ H ₆ =C ₅ H ₅ +H	5.0×10 ¹⁵	0.0	78.7	[45]
C ₅ H ₇ =C ₃ H ₄ +C ₂ H ₃	2.0×10 ¹³	0.0	54.5	estimated ^e
C ₅ H ₇ =C ₂ H ₃ +C ₃ H ₄	2.0×10 ¹³	0.0	38.1	estimated ^e
C ₅ H ₈ +O ₂ =C ₅ H ₇ +OOH	4.0×10 ¹²	0.0	60.1	estimated ^f
Reactions of aromatic species				
C ₆ H ₅ +C ₃ H ₆ =C ₆ H ₆ +C ₃ H ₅	7.9×10 ¹³	0.0	11.9	[20]
C ₆ H ₅ OH+C ₅ H ₅ =C ₆ H ₅ O+C ₅ H ₆	2.7×10 ¹⁴	0.0	25.2	[21]
C ₆ H ₅ OH+C ₃ H ₅ =C ₆ H ₅ O+C ₃ H ₆	2.7×10 ¹⁴	0.0	25.2	[21]
C ₆ H ₅ OH+C ₄ H ₅ =C ₆ H ₅ O+C ₄ H ₆	2.7×10 ¹⁴	0.0	25.2	[21]
C ₆ H ₄ OH+CH ₃ =HOC ₆ H ₄ CH ₃	5.0×10 ¹²	0.0	0.0	estimated ^d

Notes: The rate constants are given at 1 atm (—) in cm³, mol, s, kcal units.

^a -factor taken equal to that proposed by Marinov [46] and — taken equal to the enthalpy of reaction calculated by the software Thergas [17].

^bRate constant taken equal to that of C₂H₃+O₂=HCHO+CHO [47].

^cRate constant taken equal to that of the similar reaction for benzene [22].

^dRate constants of unimolecular initiations or combinations calculated using software KINGAS [25].

^e -factor taken equal to that proposed by Heyberger *et al.* [48] and activation energy estimated using the Evans-Polanyi correlation proposed by Sirjean *et al.* [31] for β-scissions of alkyl radicals.

^fRate constant of this bimolecular initiation with oxygen molecule has been calculated as proposed by Ingham *et al.* [26] with — taken equal to the enthalpy of reaction calculated by the software Thergas [14] based on the group additivity methods proposed by Benson [15].

Table S2: Added secondary mechanisms of the oxidation of ethylbenzene

Reactions	A	n	E _a	References
Added reactions of styrene				
styrene+HO2=>C6H5CH2CHO+OH	1.0x10 ¹²	0.0	14.2	estimated ^a
styrene+HO2=>C6H5COCH3+OH	1.0x10 ¹²	0.0	14.2	estimated ^a
styrene+O=C6H5CH2CHO	1.5x10 ⁸	1.45	0.9	estimated ^b
styrene+O=C6H5COCH3	1.5x10 ⁸	1.45	0.9	estimated ^b
Reactions of cumene				
<i>Unimolecular initiation</i>				
C6H5+iC3H7=cumene	1.0x10 ¹²	0.0	0.0	estimated ^c
<i>Bimolecular initiation</i>				
cumene+O2=>CH3styre+H+HO2	1.4x10 ¹²	0.0	33.6	estimated ^d
cumene+O2=C9H11-1+HO2	2.4x10 ¹³	0.0	52.3	estimated ^d
<i>Metatheses</i>				
cumene+O=OH+C9H11-1	1.0x10 ¹⁴	0.0	7.85	estimated ^e
cumene+H=H2+C9H11-1	5.7x10 ⁷	2.0	7.70	estimated ^e
cumene+OH=H2O+C9H11-1	5.3x10 ⁶	2.0	0.45	estimated ^e
cumene+HO2=H2O2+C9H11-1	1.2x10 ¹²	0.0	17.0	estimated ^e
cumene+CH3=CH4+C9H11-1	6.0x10 ⁻¹	4.0	8.2	estimated ^e
cumene+O=>OH+CH3styre+H	2.1x10 ¹¹	0.0	0.0	estimated ^f
cumene+H=>H2+CH3styre+H	9.7x10 ⁵	2.37	5.81	estimated ^g
cumene+OH=>H2O+CH3styre+H	1.7x10 ⁹	1.0	0.87	estimated ^f
cumene+OOH=>H2O2+CH3styre+H	1.3x10 ¹¹	0.0	14.0	estimated ^f
cumene+CH3=>CH4+CH3styre+H	1.3	3.76	6.98	estimated ^g
<i>Decomposition</i>				
C9H11-1=styrene+CH3	2.0x10 ¹³	0.0	31.0	estimated ^a
C9H11-1=C3H6+C6H5	2.0x10 ¹³	0.0	38.5	estimated ^a
C9H11-1=CH3styre+R1H	1.6x10 ¹³	0.0	34.3	estimated ^a
C9H11-1+O2=CH3styre+HO2	7.5x10 ¹⁰	0.0	2.5	estimated ^a
C9H11-1+H=cumene	1.0x10 ¹⁴	0.0	0.0	estimated ^h
Reactions of methylstyrene (CH3styre)				
<i>Unimolecular initiation</i>				
C6H5C2H2+R4CH3=CH3styre	4.0x10 ¹¹	0.0	0.0	estimated ^c
<i>Bimolecular initiation</i>				
CH3styre+O2=>C3H4+C6H5+HO2	1.2x10 ¹³	0.0	49.0	estimated ^d
<i>Metatheses</i>				
CH3styre+H=C2H3C6H4CH2+H2	1.7x10 ⁵	2.5	2.5	estimated ^a
CH3styre+OH=C2H3C6H4CH2+H2O	3.0x10 ⁶	2.0	-0.3	estimated ^a
CH3styre+O=>OH+C3H4+C6H5	5.1x10 ¹³	0.0	7.85	estimated ^e
CH3styre+H=>H2+C3H4+C6H5	2.8x10 ⁷	2.0	7.70	estimated ^e
CH3styre+OH=>H2O+C3H4+C6H5	2.7x10 ⁶	2.0	0.45	estimated ^e
CH3styre+HO2=>H2O2+C3H4+C6H5	6.0x10 ¹¹	0.0	17.0	estimated ^e
CH3styre+CH3=>CH4+C3H4+C6H5	3.0x10 ⁻¹	4.0	8.2	estimated ^e
Reactions of benzofuran				
C6H5O+C2H2=>benzofuran+H	1.2x10 ¹⁰	0.0	0.46	estimated ⁱ
C8H8O+H=C6H5O+C2H4	5.7x10 ¹⁰	1.43	5.65	estimated ^g
C8H7O+H=C8H8O	1.0x10 ¹⁴	0.0	0.0	estimated ^h
C8H8O+H=C8H7O+H2	9.6x10 ⁶	2.0	5.0	estimated ^e
C8H8O+O=C8H7O+OH	1.6x10 ¹³	0.0	5.2	estimated ^e
C8H8O+OH=C8H7O+H2O	2.6x10 ⁶	2.0	-0.77	estimated ^e
C8H8O+CH3=C8H7O+CH4	2.0x10 ¹¹	0.0	9.6	estimated ^e
C8H8O+H=C8H7O-1+H2	8.0x10 ¹³	0.0	6.4	estimated ^j
C8H8O+O=C8H7O-1+OH	4.2x10 ¹¹	0.0	-2.0	estimated ^j
C8H8O+OH=C8H7O-1+H2O	3.5x10 ⁹	1.0	-1.13	estimated ^j
C8H8O+CH3=C8H7O-1+CH4	1.1x10 ¹²	0.0	9.1	estimated ^j
C8H7O=benzofuran+H	3.3x10 ¹⁰	0.88	35.7	estimated ^k
C8H7O-1+H=C8H8O	1.0x10 ¹⁴	0.0	0.0	estimated ^h
C8H7O-1=benzofuran+H	1.2x10 ¹¹	0.98	42.2	estimated ^g
C8H7O+O2=benzofuran+HO2	1.6x10 ¹²	0.0	5.0	estimated ^a
C8H7O-1+O2=benzofuran+HO2	1.6x10 ¹²	0.0	15.2	estimated ^a
benzofuran+OH=>C6H4CH3+CO2	1.4x10 ¹²	0.0	-1.04	estimated ^l
benzofuran+OH=>C6H5CO+HCHO	1.4x10 ¹²	0.0	-1.04	estimated ^l
benzofuran+O=>C6H5CO+CO+H	6.0x10 ⁴	2.56	-1.13	estimated ^l

Reactions of acetophenone

<chem>C6H5COCH3+H=>H2+CH2CO+C6H5</chem>	2.8×10^7	2.0	7.70	estimated ^e
<chem>C6H5COCH3+OH=>H2O+CH2CO+C6H5</chem>	5.3×10^6	2.0	0.45	estimated ^e
<chem>C6H5COCH3+HO2=>H2O2+CH2CO+C6H5</chem>	6.0×10^{11}	0.0	17.0	estimated ^e
<chem>C6H5COCH3+CH3=>CH4+CH2CO+C6H5</chem>	3.0×10^{-1}	4.0	8.2	estimated ^e

Reactions of benzeneacetaldehyde

<chem>C6H5CH2CHO+H=>H2+CO+benzyl</chem>	4.0×10^{13}	0.0	4.2	estimated ^m
<chem>C6H5CH2CHO+OH=>H2O+CO+benzyl</chem>	4.2×10^{12}	0.0	0.5	estimated ^m
<chem>C6H5CH2CHO+OOH=>H2O2+CO+benzyl</chem>	1.0×10^{12}	0.0	10.0	estimated ^m
<chem>C6H5CH2CHO+CH3=>CH4+CO+benzyl</chem>	2.0×10^{-6}	0.0	2.5	estimated ^m
<chem>C6H5CH2CHO+C2H5=>C2H6+CO+benzyl</chem>	1.3×10^{12}	0.0	8.5E3	estimated ^m

Notes: The rate constants are given at 1 atm (—) in cm³, mol, s, kcal units.

- a: Rate constant taken equal to that proposed by Touchard et al. [37][49] in the case of alkenes, allylic and alkenyl radicals.
- b: Estimated from the rate constant of the addition of O atoms to 1,3-butadiene [11].
- c: Rate constants of unimolecular initiations or combinations calculated using software KINGAS [25].
- d: Rate constant of this bimolecular initiation with oxygen molecule has been calculated as proposed by Ingham *et al.* [26] with taken equal to the enthalpy of reaction calculated by the software Thergas [14] based on the group additivity methods proposed by Benson [15].
- e: Rate constants taken equal to the values proposed by Buda et al. [27] in the case of the similar reactions in models of alkanes oxidation.
- f: Rates constant taken equal to that of the similar reaction of toluene [8] taking into account the number abstractable H atoms.
- g: Rate constant taken equal to that theoretically calculated with CBS-QB3 method with Gaussssian03 [17] by Tian *et al.* in the case of toluene [22] taking into account the number abstractable H atoms.
- h: Rate constant taken equal to that of the recombination of H atoms with alkyl radicals as proposed by Allara and Shaw [50].
- i: Rate constant taken equal to that of the addition of OH radicals to acetylene as proposed by Baulch et al. [51].
- j: Rate constant taken equal to that of the similar reaction in the case of toluene [8] with A multiplied by 2/3 to take into account the number abstractable H atoms and with an activation energy 2 kcal/mol lower due to the abstraction of secondary H atoms instead of primary ones.
- k: Rate constant taken equal to that proposed in the case of indanyl radicals [35].
- l: Rate constant taken equal to that proposed by Heyberger *et al.* for addition to alkenes [48].
- m: Estimated as in the case of the reactions of aldehydes in the secondary mechanisms generated by EXGAS [25].

Table S3: Other changes in the primary mechanism of the oxidation of benzene and toluene for better reproducing low temperature reactivity (see description in [23]).

Reactions	A	n	E _a	References	n ^o
C6H5+O2=>C6H5O2	1.86x10 ¹³	-0.22	-0.71	[52]	(1)
C6H5O2=>C6H5+O2	6.36x10 ¹⁹	-1.37	48.74	[52]	(2)
C6H5O2=>C6H5O+O	1.27x10 ¹⁵	-0.25	38.54	[52]	(3)
C6H5O2+OOH=C6H5OOH+O2	2.0x10 ¹¹	0.0	-1.3	Estimated ^a	(4)
C6H5OOH=C6H5O+OH	1.5x10 ¹⁶	0.0	43.0	Estimated ^a	(5)
toluene+O2=benzyl+HO2	1.8x10 ¹²	0.0	39.7	[51]	(6)
toluene+CH3O=benzyl+CH3OH	2.12x10 ¹⁰	0.0	3.0	[52]	(7)
toluene+CH3OO=benzyl+CH3OOH	1.02x10 ⁴	2.5	12.3	[52]	(8)
toluene+C6H5O2=benzyl+C6H5OOH	1.02x10 ⁴	2.5	12.3	Estimated ^b	(9)
benzyl+CH3OO=>C6H5CH2O+CH3O	5.0x10 ¹²	0.0	0.0	Estimated ^c	(10)
benzyl+C2H5OO=>C6H5CH2O+C2H5O	5.0x10 ¹²	0.0	0.0	Estimated ^c	(11)
benzyl+HO2=C6H5CH2OOH	8.21x10 ⁴	2.2	-5.13	[54]	(12)
C6H5CH2OOH=C6H5CH2O+OH	3.29x10 ¹³	0.42	39.9	[54]	(13)
C6H5CH2OOH=C6H5CHO+H2O	7.45x10 ⁸	1.19	46.04	[54]	(14)
C6H5CH2O=R1H+C6H5CHO	5.26x10 ²⁸	-5.08	22.2	[55]	(15)
C6H5CH2O=C6H6#+R5CHO	2.37x10 ³²	-6.09	28.8	[55]	(16)
C6H5CH2O=C6H5#+HCHO	7.21x10 ³³	-6.21	36.8	[55]	(17)
C6H4CH3+O2=>OOC6H4CH3	3.72x10 ¹³	-0.22	-0.71	[52]	(18)
OOC6H4CH3=>C6H4CH3+O2	6.36x10 ¹⁹	-1.37	48.74	[52]	(19)
OOC6H4CH3=>OC6H4CH3+O	1.27x10 ¹⁵	-0.25	38.5	[52]	(20)
C6H5CH2OO+H=C6H5CH2O+OH	3.8x10 ¹⁴	-0.19	1.89	[56]	(21)
C6H5CH2OO+H=C6H5CH2OOH	4.35x10 ⁶⁰	-15.9	11.4	[56]	(22)
C6H5CH2OO+H=benzyl+HO2	1.96x10 ⁴	2.47	1.43	[56]	(23)

Notes: The rate constants are given at 1 atm ($k = AT^n \exp(-E_a/RT)$) in cm³, mol, s, kcal units.

^a Rate constants taken equal to the values proposed by Buda et al. [27] in the case of the similar reactions in models of alkanes oxidation.

^b Rate constants of unimolecular initiations or combinations calculated using software KINGAS [25].

^c: Rate constant taken equal to that of reaction (5).

Table S4: Reactions modified in the secondary mechanisms of toluene (see description in [23]).

Reactions	A	n	E _a	References	n ^o
Reactions modified in the secondary mechanism toluene					
C6H5CHO+CH3=C6H5CO+CH4	2.0x10 ⁻⁶	5.6	2.5	estimated ^a	(24)
C6H5CHOH=C6H5CHO+H	2.0x10 ¹³	0.0	36.3	estimated ^b	(25)
bibenzyl+H=C6H6+C8H9-1	5.6x10 ⁸	1.43	5.65	estimated ^c	(26)
bibenzyl+OH=C6H5OH+C8H9-1	7.8x10 ²	2.88	3.2	estimated ^d	(27)
C14H13+O2= stilbene+HO2	1.6x10 ¹²	0.00	15.2	estimated ^e	(28)
C14H13+OOH=>R2OH+C6H5CHO+benzyl C14H13 is C6H5•CHCH2C6H5	8.2x10 ⁴	2.20	-5.13	estimated ^f	(29)
Added submechanism for stilbene (C6H5CHCHC6H5)					
stilbene+H=>C6H6+C2H2+C6H5	5.7x10 ⁸	1.43	5.65	estimated ^c	(30)
stilbene+OH=C6H5OH+C6H5C2H2	7.8x10 ²	2.88	3.2	estimated ^d	(31)
stilbene+OH=C6H5CHO+benzyl	1.0x10 ¹³	0.0	5.9	estimated ^g	(32)
Added submechanism for phenylbenzyl ether (C6H5OCH2C6H5)					
C6H5CH2O+toluene=C6H5OCH2C6H5+CH3	7.8x10 ²	2.88	3.22	estimated ^d	(33)
C6H5O+benzyl=C6H5OCH2C6H5	1.0x10 ¹¹	0.0	0.00	estimated ⁱ	(34)
C6H5OCH2C6H5+H=C6H5CH2O+C6H6	8.5x10 ¹²	0.0	5.81	Estimated ^h	(35)
C6H5OCH2C6H5+OH=>C6H5+C6H5CHO+H2O	3.5x10 ⁹	1.0	0.87	estimated ^j	(36)
C6H5OCH2C6H5+H=>C6H5+C6H5CHO+H2	1.95x10 ⁶	2.37	5.81	estimated ^c	(37)
C6H5OCH2C6H5+O=>C6H5+C6H5CHO+OH	4.2x10 ¹¹	0.0	0.00	estimated ^j	(38)
Added submechanism for methylphenylbenzylether (To1OCH2C6H5)					
OC6H4CH3+benzyl=To1OCH2C6H5	1.0x10 ¹¹	0.0	0.00	estimated ⁱ	(39)
C6H4CH3+C6H5CH2O=To1OCH2C6H5	1.0x10 ¹¹	0.0	0.00	estimated ⁱ	(40)
To1OCH2C6H5+H=toluene+C6H5CH2O	8.5x10 ¹²	0.0	5.81	Estimated ^h	(41)
To1OCH2C6H5+OH=>C6H4CH3+C6H5CHO+H2O	8.7x10 ¹¹	1.0	0.87	estimated ^j	(42)
To1OCH2C6H5+H=>C6H4CH3+C6H5CHO+H2	4.9x10 ⁶	2.37	5.81	estimated ^c	(44)
To1OCH2C6H5+O=>C6H4CH3+C6H5CHO+OH	1.0x10 ¹²	0.0	0.00	estimated ^j	(44)
Added submechanism for ethylphenylphenol (PhenolC2H4bz)					
bibenzyl+OH=PhenolC2H4bz+H	1.7x10 ¹³	0.0	10.6	estimated ^k	(45)
C6H4OH+C8H9-1=PhenolC2H4bz	1.0x10 ¹¹	0.0	0.00	estimated ⁱ	(46)
HOC6H4CH2+benzyl=PhenolC2H4bz	1.0x10 ¹¹	0.0	0.00	estimated ⁱ	(47)
PhenolC2H4bz+OH=>styrene+C6H5O+H2O	8.7x10 ⁹	1.0	0.87	estimated ^j	(48)
PhenolC2H4bz+H=>styrene+C6H5O+H2	4.9x10 ⁶	2.37	5.81	estimated ^c	(49)
PhenolC2H4bz+O=>styrene+C6H5O+OH	1.0x10 ¹²	0.0	0.0	estimated ^j	(50)
Added submechanism for 1-butenylbenzene (C6H5C4H7)					
benzyl+C3H5=C6H5C4H7	5.0x10 ¹²	0.00	0.00	estimated ⁱ	(51)
C6H5C4H7+OH=>benzyl+pC3H4+H2O	5.2x10 ⁹	1.0	0.87	estimated ^j	(52)
C6H5C4H7+H=>benzyl+pC3H4+H2	2.9x10 ⁶	2.37	5.81	estimated ^c	(53)
C6H5C4H7+O=>benzyl+pC3H4+OH	6.3x10 ¹¹	0.0	0.0	estimated ^j	(54)
C6H5C4H7+OH=>benzyl+pC3H4+H2O	3.0x10 ⁶	2.0	-1.52	estimated ^e	(55)
C6H5C4H7+H=>benzyl+pC3H4+H2	5.4x10 ⁴	2.5	-1.9	estimated ^e	(56)
C6H5C4H7+O=>benzyl+pC3H4+OH	8.8x10 ¹⁰	0.7	3.25	estimated ^e	(57)

Notes: The rate constants are given at 1 atm (—) in cm³, mol, s, kcal units.

a: Rate constant taken equal to that proposed by Baulch *et al.* [57] for acetaldehyde.

b: -factor taken equal to that proposed Heyberger *et al.* [48] and activation energy estimated using the Evans-Polyanyi correlation proposed by Sirjean *et al.* [31] for β-scissions of alkyl radicals.

c: Rate constant taken equal to that theoretically calculated with CBS-QB3 method with Gaussian03 [17] by Tian *et al.* [22], with when needed A-factor multiplied by a factor taking into account the number abstractable H atoms.

- d: Rate constant taken equal to that of the similar reaction of toluene proposed by Seta *et al.* [58].
- e: Rate constant taken equal to that proposed by Touchard *et al.* [37] in the case of allylic radicals.
- f: Rate constant taken equal to that used for the similar reaction of benzyl radicals [54].
- g: Rate constant taken equal to that of the similar reaction for ethylene proposed by Baulch *et al.* [57].
- h: Rate constant taken equal to that proposed by Manion and Louw [59] for the same reaction for phenol.
- i: Rate constants of unimolecular initiations or combinations calculated using software KINGAS [25].
- j: Rate constant taken equal to that of the similar reaction in the case of toluene [8] with A-factor multiplied by a factor taking into account the number abstractable H atoms.
- k: Rate constant taken equal to that of the similar reaction in the case of toluene [8].

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