

Annex 1.

Primary propagation reactions of n-decane oxidation

(Units are kcal, kmole, m, s, K)

Initiation reactions

		A	E
C-C-C-C-C-C-C-C-C-C	\Rightarrow C* + *C-C-C-C-C-C-C-C	1.00E+17	83000
C-C-C-C-C-C-C-C-C-C	\Rightarrow C-C* + *C-C-C-C-C-C-C	1.00E+17	81000
C-C-C-C-C-C-C-C-C-C	\Rightarrow C-C-C* + *C-C-C-C-C-C	1.00E+17	81000
C-C-C-C-C-C-C-C-C-C	\Rightarrow C-C-C-C* + *C-C-C-C-C	1.00E+17	81000
C-C-C-C-C-C-C-C-C-C	\Rightarrow C-C-C-C-C* + *C-C-C-C	0.50E+17	81000

H-abstraction reactions

R* + C-C-C-C-C-C-C-C-C	\Rightarrow *C-C-C-C-C-C-C-C	6 primary	H atoms
R* + C-C-C-C-C-C-C-C-C	\Rightarrow C-*C-C-C-C-C-C-C-C	4 secondary	H atoms
R* + C-C-C-C-C-C-C-C-C	\Rightarrow C-C-*C-C-C-C-C-C-C	4 secondary	H atoms
R* + C-C-C-C-C-C-C-C-C	\Rightarrow C-C-C-*C-C-C-C-C-C	4 secondary	H atoms
R* + C-C-C-C-C-C-C-C-C	\Rightarrow C-C-C-C-*C-C-C-C-C	4 secondary	H atoms

β -decomposition of alkyl radical

*C-C-C-C-C-C-C-C-C-C	\Rightarrow C=C + *C-C-C-C-C-C	1.00E+14	30000
C-*C-C-C-C-C-C-C-C	\Rightarrow C-C=C + *C-C-C-C-C	1.00E+14	31000
C-C-*C-C-C-C-C-C-C	\Rightarrow C=C-C-C-C-C-C + *C	1.00E+14	33000
C-C-*C-C-C-C-C-C-C	\Rightarrow C-C-C=C + *C-C-C-C	1.00E+14	31000
C-C-C-*C-C-C-C-C-C	\Rightarrow C=C-C-C-C-C-C + C-*C	1.00E+14	31000
C-C-C-*C-C-C-C-C-C	\Rightarrow C-C-C-C=C + *C-C-C-C	1.00E+14	31000
C-C-C-C-*C-C-C-C-C	\Rightarrow C=C-C-C-C-C + C-C-*C	1.00E+14	31000
C-C-C-C-*C-C-C-C-C	\Rightarrow C-C-C-C=C + *C-C-C-C	1.00E+14	31000

Isomerization (H-transfer) of alkyl radical

*C-C-C-C-C-C-C-C-C-C	\Rightarrow C-C-C-*C-C-C-C-C	1.89E+11	18300
*C-C-C-C-C-C-C-C-C	\Rightarrow C-C-C-*C-C-C-C-C	3.00E+10	12200
*C-C-C-C-C-C-C-C-C	\Rightarrow C-C-C-*C-C-C-C-C	1.20E+10	12200
C-*C-C-C-C-C-C-C-C	\Rightarrow C-C-C-*C-C-C-C-C	1.89E+11	19300
C-*C-C-C-C-C-C-C-C	\Rightarrow C-C-C-*C-C-C-C-C	3.00E+10	13200
C-*C-C-C-C-C-C-C-C	\Rightarrow C-C-C-*C-C-C-C-C	1.20E+10	13200
C-C-*C-C-C-C-C-C-C	\Rightarrow C-C-C-*C-C-C-C-C	1.89E+11	19300
C-C-*C-C-C-C-C-C-C	\Rightarrow C-C-C-*C-C-C-C-C	3.00E+10	13200
C-C-*C-C-C-C-C-C-C	\Rightarrow C-C-*C-C-C-C-C-C	1.20E+10	13200
C-C-C-*C-C-C-C-C-C	\Rightarrow *C-C-C-C-C-C-C-C	2.84E+11	21600
C-C-C-*C-C-C-C-C-C	\Rightarrow C-C-C-*C-C-C-C-C	1.89E+11	19300
C-C-C-*C-C-C-C-C-C	\Rightarrow C-C-*C-C-C-C-C-C	3.00E+10	13200
C-C-C-*C-C-C-C-C-C	\Rightarrow C-*C-C-C-C-C-C-C	1.20E+10	13200
C-C-C-*C-C-C-C-C-C	\Rightarrow C-*C-C-C-C-C-C-C	1.89E+11	19300
C-C-C-C-*C-C-C-C-C	\Rightarrow C-C-*C-C-C-C-C-C	1.89E+11	19300
C-C-C-C-*C-C-C-C-C	\Rightarrow *C-C-C-C-C-C-C-C	4.50E+10	15500
C-C-C-C-*C-C-C-C-C	\Rightarrow C-*C-C-C-C-C-C-C	3.00E+10	13200
C-C-C-C-*C-C-C-C-C	\Rightarrow *C-C-C-C-C-C-C-C	1.80E+10	15500

O₂ abstractions on of alkyl radicals to form HO₂[·] and conjugate alkenes

*C-C-C-C-C-C-C-C-C + O ₂	\Rightarrow C=C-C-C-C-C-C-C + HO ₂	3.00E+08	3500
C-*C-C-C-C-C-C-C-C + O ₂	\Rightarrow C=C-C-C-C-C-C-C + HO ₂	4.50E+08	3500
C-*C-C-C-C-C-C-C-C + O ₂	\Rightarrow C-C=C-C-C-C-C-C + HO ₂	3.00E+08	3500
C-C-*C-C-C-C-C-C-C + O ₂	\Rightarrow C-C=C-C-C-C-C-C + HO ₂	3.00E+08	3500
C-C-*C-C-C-C-C-C-C + O ₂	\Rightarrow C-C=C-C-C-C-C-C + HO ₂	3.00E+08	3500
C-C-C-*C-C-C-C-C-C + O ₂	\Rightarrow C-C=C-C-C-C-C-C + HO ₂	3.00E+08	3500
C-C-C-*C-C-C-C-C-C + O ₂	\Rightarrow C-C=C-C-C-C-C-C + HO ₂	3.00E+08	3500

C-C-C-C-*C-C-C-C-C-C + O2	\Rightarrow	C-C-C-C=C-C-C-C-C-C + HO2	3.00E+08	3500
C-C-C-C-*C-C-C-C-C-C + O2	\Rightarrow	C-C-C-C=C-C-C-C-C-C + HO2	3.00E+08	3500

O₂ addition on alkyl radicals to form peroxy radicals (and reverse reactions)

C-C-C-C-C-C-C-C-C-C + O2	\Rightarrow	COO-C-C-C-C-C-C-C-C-C	1.00E+09	0
COO*-C-C-C-C-C-C-C-C-C	\Rightarrow	*C-C-C-C-C-C-C-C-C-C + O2	3.00E+13	30000
C-*C-C-C-C-C-C-C-C-C + O2	\Rightarrow	C-COO*-C-C-C-C-C-C-C-C	1.00E+09	0
C-COO*-C-C-C-C-C-C-C-C	\Rightarrow	*C-C-C-C-C-C-C-C-C-C + O2	3.00E+13	30000
C-C-*C-C-C-C-C-C-C-C + O2	\Rightarrow	C-C-COO*-C-C-C-C-C-C-C	1.00E+09	0
C-C-COO*-C-C-C-C-C-C-C	\Rightarrow	C-C-*C-C-C-C-C-C-C + O2	3.00E+13	30000
C-C-C-*C-C-C-C-C-C + O2	\Rightarrow	C-C-C-COO*-C-C-C-C-C-C	1.00E+09	0
C-C-C-C-COO*-C-C-C-C-C	\Rightarrow	C-C-C-C-*C-C-C-C-C-C + O2	3.00E+13	30000

Isomerization of ROO[·] to QOOH radicals

COO*-C-C-C-C-C-C-C-C-C	\Rightarrow	COOH-*C-C-C-C-C-C-C-C-C	1.26E+12	26800
COO*-C-C-C-C-C-C-C-C-C	\Rightarrow	COOH-C-*C-C-C-C-C-C-C-C	2.00E+11	20700
COO*-C-C-C-C-C-C-C-C-C	\Rightarrow	COOH-C-C-*C-C-C-C-C-C-C	8.00E+10	20700
C-COO*-C-C-C-C-C-C-C-C	\Rightarrow	*C-COOH-C-C-C-C-C-C-C-C	1.89E+12	29100
C-COO*-C-C-C-C-C-C-C-C	\Rightarrow	C-COOH-*C-C-C-C-C-C-C-C	1.26E+12	26800
C-COO*-C-C-C-C-C-C-C-C	\Rightarrow	C-COOH-C-*C-C-C-C-C-C-C	2.00E+11	20700
C-COO*-C-C-C-C-C-C-C-C	\Rightarrow	C-COOH-C-C-*C-C-C-C-C-C	8.00E+10	20700
C-C-COO*-C-C-C-C-C-C-C	\Rightarrow	C-*C-COOH-C-C-C-C-C-C-C	1.26E+12	26800
C-C-COO*-C-C-C-C-C-C-C	\Rightarrow	C-C-COOH-*C-C-C-C-C-C-C	1.26E+12	26800
C-C-COO*-C-C-C-C-C-C-C	\Rightarrow	*C-C-COOH-C-C-C-C-C-C-C	3.00E+11	23000
C-C-COO*-C-C-C-C-C-C-C	\Rightarrow	C-C-COOH-C-*C-C-C-C-C-C	2.00E+11	20700
C-C-COO*-C-C-C-C-C-C-C	\Rightarrow	C-C-COOH-C-C-*C-C-C-C-C	8.00E+10	20700
C-C-C-COO*-C-C-C-C-C-C	\Rightarrow	C-C-*C-COOH-C-C-C-C-C-C	1.26E+12	26800
C-C-C-COO*-C-C-C-C-C-C	\Rightarrow	C-C-C-COOH-*C-C-C-C-C-C	1.26E+12	26800
C-C-C-COO*-C-C-C-C-C-C	\Rightarrow	C-C-C-COOH-C-C-C-C-C-C	2.00E+11	20700
C-C-C-C-COO*-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	1.26E+12	26800
C-C-C-C-COO*-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	2.00E+11	20700
C-C-C-C-COO*-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	8.00E+10	20700
C-C-C-C-COO*-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	8.00E+10	20700

Isomerization of QOOH to ROO[·] to radicals

COOH-*C-C-C-C-C-C-C-C-C	\Rightarrow	COO*-C-C-C-C-C-C-C-C-C	9.45E+10	19100
COOH-C-*C-C-C-C-C-C-C-C	\Rightarrow	COO*-C-C-C-C-C-C-C-C-C	1.50E+10	13000
COOH-C-C-*C-C-C-C-C-C-C	\Rightarrow	COO*-C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-COOH-C-C-C-C-C-C-C-C	\Rightarrow	C-COO-C-C-C-C-C-C-C-C	9.45E+10	18100
C-COOH-*C-C-C-C-C-C-C-C	\Rightarrow	C-COO*-C-C-C-C-C-C-C-C	9.45E+10	19100
C-COOH-C-*C-C-C-C-C-C-C	\Rightarrow	C-COO*-C-C-C-C-C-C-C-C	1.50E+10	13000
C-COOH-C-C-*C-C-C-C-C-C	\Rightarrow	C-COO*-C-C-C-C-C-C-C-C	6.00E+09	13000
C-C-COOH-C-C-C-C-C-C-C	\Rightarrow	C-C-C-COO-C-C-C-C-C-C	1.50E+10	12000
C-C-C-COOH-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-*C-C-C-C-C	9.45E+10	19100
C-C-C-C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	2.00E+11	20700
C-C-C-C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	2.00E+11	20700
C-C-C-C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	8.00E+10	20700
C-C-C-C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	8.00E+10	20700
C-C-C-C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	1.50E+10	13000
C-C-C-C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	6.00E+09	13000
*C-C-C-COOH-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-*C-C-C-C-C	6.00E+09	12000
C-C-C-C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	1.50E+10	13000
C-C-C-C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	9.45E+10	19100
C-C-C-C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	9.45E+10	19100
C-C-C-C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	1.50E+10	13000
C-C-C-C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	6.00E+09	13000
C-C-C-C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	6.00E+09	13000
C-C-C-C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-C-C-COOH-C-C-C-C-C	1.50E+10	13000

C-C-C- * C-COOH-C-C-C-C-C	\Rightarrow	C-C-C-C-COO * -C-C-C-C-C	9.45E+10	19100
C-C-C-C-COOH- * C-C-C-C-C	\Rightarrow	C-C-C-C-COO * -C-C-C-C-C	9.45E+10	19100
C-C-C-C-COOH-C- * C-C-C-C	\Rightarrow	C-C-C-C-COO * -C-C-C-C-C	1.50E+10	13000
C-C-C-C-COOH-C-C- * C-C-C	\Rightarrow	C-C-C-C-COO * -C-C-C-C-C	6.00E+09	13000

Decomposition of 'QOOH radicals to form small alkenes and aldehydes

COOH-C-*C-C-C-C-C-C-C-C	\Rightarrow	CO + C=C-C-C-C-C-C-C + OH	1.50E+13	22500
C-COOH-C-*C-C-C-C-C-C-C	\Rightarrow	C-CO + C=C-C-C-C-C-C + OH	1.50E+13	22500
*C-C-COOH-C-C-C-C-C-C-C	\Rightarrow	CO-C-C-C-C-C-C-C + C=C + OH	1.50E+13	22500
C-C-COOH-C-*C-C-C-C-C-C	\Rightarrow	C-C-CO + C=C-C-C-C-C-C + OH	1.50E+13	22500
C-*C-C-COOH-C-C-C-C-C-C	\Rightarrow	CO-C-C-C-C-C-C-C + C-C=C + OH	1.50E+13	22500
C-C-C-COOH-C-*C-C-C-C-C	\Rightarrow	C-C-C-CO + C=C-C-C-C-C + OH	1.50E+13	22500
C-C-*C-C-COOH-C-C-C-C-C	\Rightarrow	CO-C-C-C-C-C + C-C-C=C + OH	1.50E+13	22500
C-C-C-C-COOH-C-*C-C-C-C	\Rightarrow	C-C-C-C-CO + C=C-C-C-C + OH	1.50E+13	22500

Decomposition of 'QOOH radicals to form HO₂[.] and conjugate alkenes

COOH-*C-C-C-C-C-C-C-C-C-C	\Rightarrow	C=C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
*C-COOH-C-C-C-C-C-C-C-C	\Rightarrow	C=C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-COOH-*C-C-C-C-C-C-C-C	\Rightarrow	C-C=C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-*C-COOH-C-C-C-C-C-C-C	\Rightarrow	C-C=C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-COOH-*C-C-C-C-C-C-C	\Rightarrow	C-C=C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-*C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-C=C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-COOH-*C-C-C-C-C-C	\Rightarrow	C-C-C=C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-*C-COOH-C-C-C-C-C	\Rightarrow	C-C-C-C=C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-C-COOH-*C-C-C-C-C	\Rightarrow	C-C-C-C=C-C-C-C-C + HO2	1.00E+14	23000

Decomposition of 'QOOH radicals to form cyclic ethers and OH

COOH-*C-C-C-C-C-C-C-C-C-C	=> ^C-^C-C-C-C-C-C-C-C + OH	9.45E+11	18000
COOH-C-*C-C-C-C-C-C-C-C	=> ^C-C-^C-C-C-C-C-C-C + OH	1.50E+11	17000
COOH-C-C-*C-C-C-C-C-C-C	=> ^C-C-C-^C-C-C-C-C-C-C + OH	2.40E+10	8500
*C-COOH-C-C-C-C-C-C-C-C	=> ^C-^C-C-C-C-C-C-C-C + OH	9.45E+11	18000
C-COOH-*C-C-C-C-C-C-C-C	=> C-^C-^C-C-C-C-C-C-C + OH	9.45E+11	18000
C-COOH-C-*C-C-C-C-C-C-C	=> C-^C-C-^C-C-C-C-C-C + OH	1.50E+11	17000
C-COOH-C-C-*C-C-C-C-C-C	=> C-^C-C-C-^C-C-C-C-C-C + OH	2.40E+10	8500
*C-C-COOH-C-C-C-C-C-C-C	=> ^C-C-^C-C-C-C-C-C-C-C + OH	1.50E+11	17000
C-*C-COOH-C-C-C-C-C-C	=> C-^C-^C-C-C-C-C-C-C + OH	9.45E+11	18000
C-C-COOH-*C-C-C-C-C-C	=> C-C-^C-^C-C-C-C-C-C + OH	9.45E+11	18000
C-C-COOH-C-*C-C-C-C-C-C	=> C-C-^C-C-^C-C-C-C-C + OH	1.50E+11	17000
C-C-COOH-C-C-*C-C-C-C-C	=> C-C-^C-C-C-^C-C-C-C-C + OH	2.40E+10	8500
*C-C-C-COOH-C-C-C-C-C-C	=> ^C-C-C-^C-C-C-C-C-C-C + OH	2.40E+10	8500
C-*C-C-COOH-C-C-C-C-C-C	=> C-^C-C-^C-C-C-C-C-C-C + OH	1.50E+11	17000
C-C-*C-COOH-C-C-C-C-C-C	=> C-C-^C-C-^C-C-C-C-C-C + OH	9.45E+11	18000
C-C-C-COOH-*C-C-C-C-C-C	=> C-C-C-^C-^C-C-C-C-C-C + OH	9.45E+11	18000
C-C-C-COOH-C-*C-C-C-C-C	=> C-C-C-C-^C-^C-C-C-C-C + OH	1.50E+11	17000
C-C-C-C-COOH-C-*C-C-C-C	=> C-C-C-C-C-^C-^C-C-C-C + OH	2.40E+10	8500
C-C-C-C-COOH-C-C-*C-C-C	=> C-C-^C-C-C-^C-C-C-C-C + OH	2.40E+10	8500

O₂ addition on 'QOOH to form 'OOQOOH radicals (and reverse reactions)

COOH-*C-C-C-C-C-C-C-C-C +O2	\Rightarrow	COOH-COO*-C-C-C-C-C-C-C-C	1.00E+09	0
COOH-COO*-C-C-C-C-C-C-C-C	\Rightarrow	COOH-*C-C-C-C-C-C-C-C + O2	3.00E+13	30000
COOH-C-*C-C-C-C-C-C-C-C +O2	\Rightarrow	COOH-C-COO*-C-C-C-C-C-C-C	1.00E+09	0
COOH-C-COO*-C-C-C-C-C-C-C	\Rightarrow	COOH-C-*C-C-C-C-C-C-C + O2	3.00E+13	30000
COOH-C-C-*C-C-C-C-C-C-C +O2	\Rightarrow	COOH-C-C-COO*-C-C-C-C-C-C	1.00E+09	0
COOH-C-C-COO*-C-C-C-C-C-C	\Rightarrow	COOH-C-C-*C-C-C-C-C-C + O2	3.00E+13	30000
C-COOH-C-C-C-C-C-C-C +O2	\Rightarrow	COO-COOH-C-C-C-C-C-C-C	1.00E+09	0
COO*-COOH-C-C-C-C-C-C-C	\Rightarrow	*C-COOH-C-C-C-C-C-C-C + O2	3.00E+13	30000

Decomposition of 'OOQOOH radicals to form keto-hydroperoxides (OQOOH)

COOH-COO*-C-C-C-C-C-C-C-C	\Rightarrow	*CO + CO-C-C-C-C-C-C-C + 2 OH	6.30E+11	26600
COOH-C-C-COO*-C-C-C-C-C-C	\Rightarrow	CO-*C + CO-C-C-C-C-C-C + 2 OH	1.00E+11	20500
COOH-C-C-COO*-C-C-C-C-C-C	\Rightarrow	CO-C-*C + CO-C-C-C-C-C + 2 OH	4.00E+10	20500
COO*-COOH-C-C-C-C-C-C-C	\Rightarrow	*CO-C-C-C-C-C-C + CO + 2 OH	6.30E+11	26600
C-COOH-COO*-C-C-C-C-C-C	\Rightarrow	C-*CO + CO-C-C-C-C-C-C + 2 OH	6.30E+11	26600
C-COOH-C-COO*-C-C-C-C-C	\Rightarrow	C-CO-*C + CO-C-C-C-C-C + 2 OH	1.00E+11	20500
C-COOH-C-C-COO*-C-C-C-C-C	\Rightarrow	C-CO-C-*C + CO-C-C-C-C + 2 OH	4.00E+10	20500
COO*-C-COOH-C-C-C-C-C-C	\Rightarrow	*C-CO-C-C-C-C-C + CO + 2 OH	1.00E+11	20500
C-COO*-COOH-C-C-C-C-C-C	\Rightarrow	*CO-C-C-C-C-C-C + C-CO + 2 OH	6.30E+11	26600
C-C-COOH-COO*-C-C-C-C-C	\Rightarrow	C-C-*CO + CO-C-C-C-C-C + 2 OH	6.30E+11	26600
C-C-COOH-C-COO*-C-C-C-C-C	\Rightarrow	C-C-CO-*C + CO-C-C-C-C + 2 OH	1.00E+11	20500
C-C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-CO-C-*C + CO-C-C-C-C + 2 OH	4.00E+10	20500
COO*-C-C-COOH-C-C-C-C-C	\Rightarrow	*C-C-CO-C-C-C-C + CO + 2 OH	4.00E+10	20500
C-COO*-C-COOH-C-C-C-C-C	\Rightarrow	*C-CO-C-C-C-C-C + C-CO + 2 OH	1.00E+11	20500
C-C-COO*-COOH-C-C-C-C-C	\Rightarrow	*CO-C-C-C-C-C + C-C-CO + 2 OH	6.30E+11	26600
C-C-C-COOH-COO*-C-C-C-C-C	\Rightarrow	C-C-C-*CO + CO-C-C-C-C-C + 2 OH	6.30E+11	26600
C-C-C-COOH-C-COO*-C-C-C-C	\Rightarrow	C-C-C-CO-*C + CO-C-C-C-C + 2 OH	1.00E+11	20500
C-C-C-COOH-C-C-C-C-C-C	\Rightarrow	C-C-C-CO-C-*C + CO-C-C-C-C + 2 OH	4.00E+10	20500
C-C-COO*-C-C-COOH-C-C-C-C	\Rightarrow	*C-C-CO-C-C-C-C + C-C-CO + 2 OH	4.00E+10	20500
C-C-COO*-C-COOH-C-C-C-C-C	\Rightarrow	*C-CO-C-C-C-C-C + C-C-CO + 2 OH	1.00E+11	20500
C-C-C-COO*-COOH-C-C-C-C-C	\Rightarrow	*CO-C-C-C-C-C + CO-C-C-C + 2 OH	6.30E+11	26600

C-C-C-C-COOH-COO*-C-C-C-C	\Rightarrow	C-C-C-C-*CO + CO-C-C-C-C + 2 OH	6.30E+11	26600
C-C-C-C-COOH-C-C-COO*-C-C-C	\Rightarrow	C-C-C-C-CO-*C + CO-C-C-C + 2 OH	1.00E+11	20500
C-C-C-C-COOH-C-C-COO*-C-C-C	\Rightarrow	C-C-C-C-CO-C-*C + C-C-CO + 2 OH	4.00E+10	20500

Primary propagation reactions of n-dodecane oxidation

(Units are kcal, kmole, m, s, K)

Initiation reactions

		A	E
C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C^* + *C-C-C-C-C-C-C-C-C-C$	1.00E+17	83000
C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C^* + *C-C-C-C-C-C-C-C-C$	1.00E+17	81000
C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C^* + *C-C-C-C-C-C-C-C-C$	1.00E+17	81000
C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C^* + *C-C-C-C-C-C-C-C$	1.00E+17	81000
C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C^* + *C-C-C-C-C-C-C$	1.00E+17	81000
C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-C^* + *C-C-C-C-C-C$	0.50E+17	81000

H-abstraction reactions

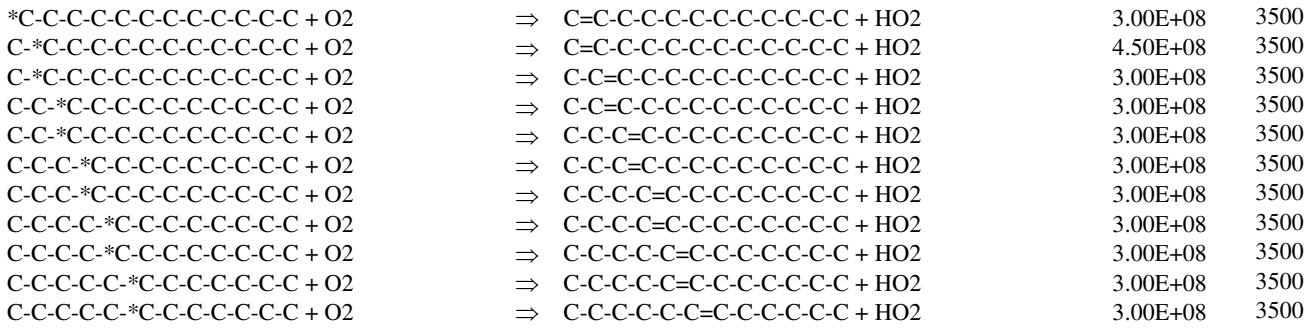
$R^* + C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow *C-C-C-C-C-C-C-C-C-C-C$	6 primary	H atoms
$R^* + C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-*C-C-C-C-C-C-C-C-C-C$	4 secondary	H atoms
$R^* + C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C-*C-C-C-C-C-C-C-C-C$	4 secondary	H atoms
$R^* + C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C-C-*C-C-C-C-C-C-C-C$	4 secondary	H atoms
$R^* + C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C-C-C-*C-C-C-C-C-C-C$	4 secondary	H atoms
$R^* + C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C-C-C-C-*C-C-C-C-C-C$	4 secondary	H atoms

β -decomposition of alkyl radical

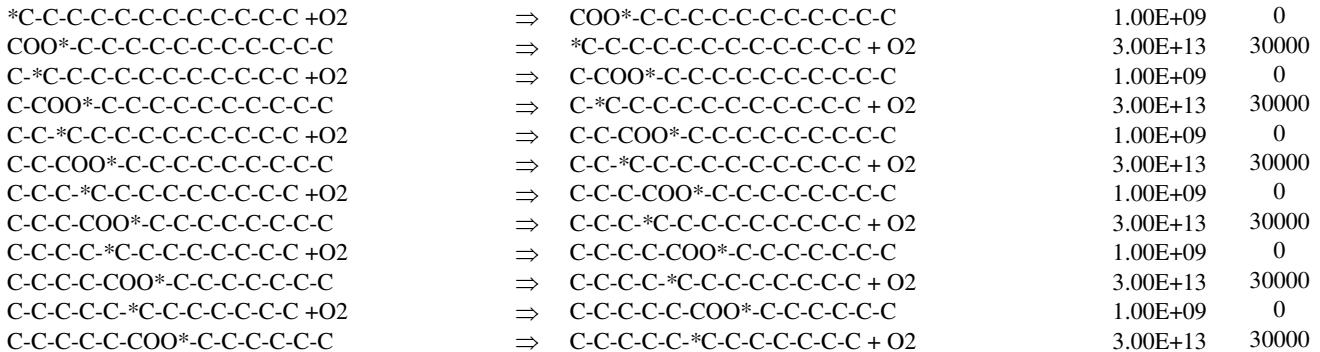
$*C-C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C=C + *C-C-C-C-C-C-C-C-C$	1.00E+14	30000
$C-*C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C=C + *C-C-C-C-C-C-C-C$	1.00E+14	31000
$C-C-*C-C-C-C-C-C-C-C-C$	$\Rightarrow C=C-C-C-C-C-C-C-C-C+C$	1.00E+14	33000
$C-C-*C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C-C=C + *C-C-C-C-C-C-C$	1.00E+14	31000
$C-C-C-*C-C-C-C-C-C-C-C$	$\Rightarrow C=C-C-C-C-C-C-C-C+C-*C$	1.00E+14	31000
$C-C-C-*C-C-C-C-C-C-C-C$	$\Rightarrow C-C-C-C=C + *C-C-C-C-C-C$	1.00E+14	31000
$C-C-C-C-*C-C-C-C-C-C-C$	$\Rightarrow C=C-C-C-C-C-C-C+C-C-*C$	1.00E+14	31000
$C-C-C-C-*C-C-C-C-C-C-C$	$\Rightarrow C-C-C-C-C=C + *C-C-C-C-C$	1.00E+14	31000
$C-C-C-C-C-*C-C-C-C-C-C$	$\Rightarrow C=C-C-C-C-C-C+C-C-C-*C$	1.00E+14	31000

Isomerization (H-transfer) of alkyl radical

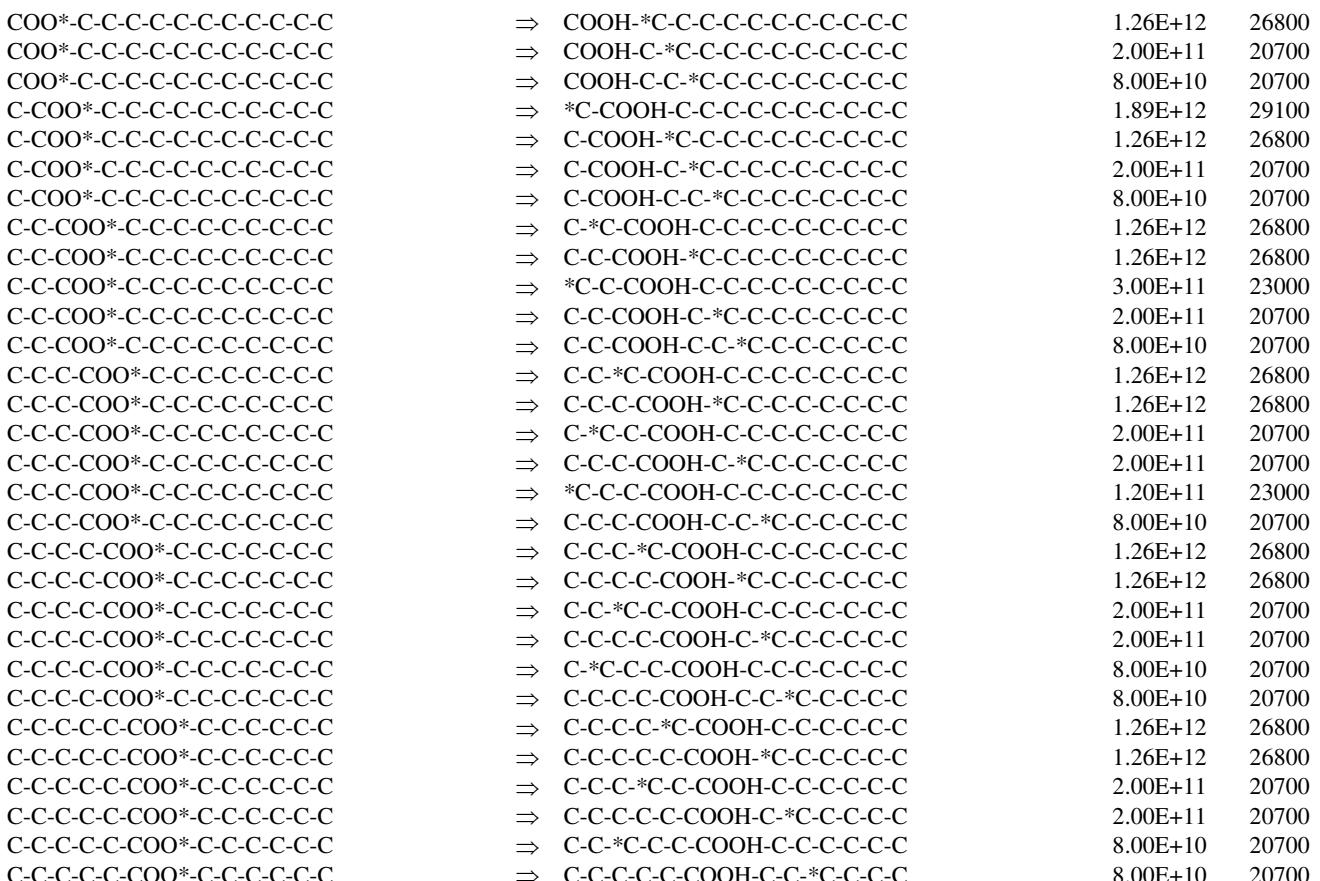
O₂ abstractions on of alkyl radicals to form HO₂[·] and conjugate alkenes



O₂ addition on alkyl radicals to form peroxy radicals (and reverse reactions)



Isomerization of ROO[·] to QOOH radicals



Isomerization of 'OOOH' to ROO' to radicals



COOH-C-*C-C-C-C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	1.50E+10	13000
COOH-C-C-*C-C-C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-COOH-C-C-C-C-C-C-C-C-C	⇒ COO-C-C-C-C-C-C-C-C-C-C	9.45E+10	18100
C-COOH-*C-C-C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-COOH-C-*C-C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-COOH-C-C-*C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-C-COOH-C-C-C-C-C-C-C-C	⇒ COO-C-C-C-C-C-C-C-C-C-C	1.50E+10	12000
C-*C-COOH-C-C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-COOH-*C-C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-COOH-C-*C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-COOH-C-C-*C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-C-C-COOH-C-C-C-C-C-C-C	⇒ COO-C-C-C-C-C-C-C-C-C-C	6.00E+09	12000
C-*C-C-COOH-C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-C-COOH-*C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-C-COOH-C-C-*C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-C-COOH-C-*C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-C-COOH-C-C-*C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-*C-C-C-COOH-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-C-C-C-COOH-*C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-C-C-COOH-C-C-*C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-C-C-COOH-C-*C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-C-C-COOH-C-C-*C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-C-C-COOH-C-C-C-*C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-C-C-C-COOH-C-C-C-C-*C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-C-C-COOH-C-C-C-C-C-*C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-C-C-COOH-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C	6.00E+09	13000

Decomposition of 'QOOH radicals to form small alkenes and aldehydes

COOH-C-*C-C-C-C-C-C-C-C-C-C	⇒ CO + C=C-C-C-C-C-C-C-C-C + OH	1.50E+13	22500
C-COOH-C-*C-C-C-C-C-C-C-C-C	⇒ C-CO + C=C-C-C-C-C-C-C-C + OH	1.50E+13	22500
*C-C-COOH-C-C-C-C-C-C-C-C-C	⇒ CO-C-C-C-C-C-C-C-C-C + C=C + OH	1.50E+13	22500
C-C-COOH-C-*C-C-C-C-C-C-C-C	⇒ C-C-CO + C=C-C-C-C-C-C-C + OH	1.50E+13	22500
C-*C-C-COOH-C-C-C-C-C-C-C-C	⇒ CO-C-C-C-C-C-C-C-C + C-C=C + OH	1.50E+13	22500
C-C-C-COOH-C-*C-C-C-C-C-C-C	⇒ C-C-C-C-C-C-C-C + C-C-C=C + OH	1.50E+13	22500
C-C-C-C-COOH-C-*C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C + C-C-C=C + OH	6.00E+09	13000
C-C-C-C-COOH-C-C-*C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C + C-C-C=C + OH	6.00E+09	13000
C-C-C-C-COOH-C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C + C-C-C=C + OH	1.50E+10	13000
C-C-C-C-COOH-C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C + C-C-C=C + OH	9.45E+10	19100
C-C-C-C-COOH-C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C + C-C-C=C + OH	9.45E+10	19100
C-C-C-C-COOH-C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C + C-C-C=C + OH	1.50E+10	13000
C-C-C-C-COOH-C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C + C-C-C=C + OH	6.00E+09	13000

Decomposition of 'QOOH radicals to form HO2' and conjugate alkenes

COOH-*C-C-C-C-C-C-C-C-C-C-C	⇒ C=C-C-C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
*C-COOH-C-C-C-C-C-C-C-C-C-C	⇒ C=C-C-C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-COOH-*C-C-C-C-C-C-C-C-C-C	⇒ C-C=C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-*C-COOH-C-C-C-C-C-C-C-C-C	⇒ C-C=C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-COOH-*C-C-C-C-C-C-C-C-C	⇒ C-C-C=C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-*C-COOH-C-C-C-C-C-C-C-C	⇒ C-C-C=C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-COOH-*C-C-C-C-C-C-C-C	⇒ C-C-C=C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-C-COOH-*C-C-C-C-C-C-C	⇒ C-C-C=C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-C-COOH-*C-C-C-C-C-C-C	⇒ C-C-C=C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-C-COOH-*C-C-C-C-C-C-C	⇒ C-C-C=C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-C-COOH-*C-C-C-C-C-C-C	⇒ C-C-C=C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-C-COOH-*C-C-C-C-C-C-C	⇒ C-C-C=C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-C-COOH-*C-C-C-C-C-C-C	⇒ C-C-C=C-C-C-C-C-C-C + HO2	1.00E+14	23000

Decomposition of 'QOOH radicals to form cyclic ethers and OH

COOH-*C-C-C-C-C-C-C-C-C-C-C	⇒ ^C-C-C-C-C-C-C-C-C-C-C + OH	9.45E+11	18000
COOH-C-*C-C-C-C-C-C-C-C-C-C	⇒ ^C-C-C-C-C-C-C-C-C-C-C + OH	1.50E+11	17000
COOH-C-C-*C-C-C-C-C-C-C-C-C	⇒ ^C-C-C-C-C-C-C-C-C-C-C + OH	2.40E+10	8500
*C-COOH-C-C-C-C-C-C-C-C-C-C	⇒ ^C-C-C-C-C-C-C-C-C-C-C + OH	9.45E+11	18000
C-COOH-*C-C-C-C-C-C-C-C-C-C	⇒ C-^C-C-C-C-C-C-C-C-C-C + OH	9.45E+11	18000
C-COOH-C-*C-C-C-C-C-C-C-C-C	⇒ C-^C-C-C-C-C-C-C-C-C-C + OH	1.50E+11	17000

O₂ addition on 'QOOH to form 'OOQOOH radicals (and reverse reactions)

Decomposition of 'OOQOOH radicals to form keto-hydroperoxides (OQOOH)

COOH-COO*-C-C-C-C-C-C-C-C-C-C	⇒ *CO + CO-C-C-C-C-C-C-C-C-C + 2 OH	6.30E+11	26600
COOH-C-COO*-C-C-C-C-C-C-C-C	⇒ CO-*C + CO-C-C-C-C-C-C-C + 2 OH	1.00E+11	20500
COOH-C-C-COO*-C-C-C-C-C-C-C	⇒ CO-C-*C + CO-C-C-C-C-C-C-C + 2 OH	4.00E+10	20500
COO*-COOH-C-C-C-C-C-C-C-C	⇒ *CO-C-C-C-C-C-C-C-C + CO + 2 OH	6.30E+11	26600
C-COOH-COO*-C-C-C-C-C-C-C	⇒ C-*CO + CO-C-C-C-C-C-C-C + 2 OH	6.30E+11	26600
C-COOH-C-COO*-C-C-C-C-C-C	⇒ C-CO-*C + CO-C-C-C-C-C-C + 2 OH	1.00E+11	20500
C-COOH-C-C-COO*-C-C-C-C-C-C	⇒ C-CO-C-*C + CO-C-C-C-C-C-C + 2 OH	4.00E+10	20500
COO*-C-COOH-C-C-C-C-C-C-C	⇒ *C-CO-C-C-C-C-C-C-C + CO + 2 OH	1.00E+11	20500
C-COO*-COOH-C-C-C-C-C-C	⇒ *CO-C-C-C-C-C-C-C + C-CO + 2 OH	6.30E+11	26600
C-C-COOH-COO*-C-C-C-C-C-C	⇒ C-C-*CO + CO-C-C-C-C-C-C + 2 OH	6.30E+11	26600
C-C-COOH-C-COO*-C-C-C-C-C-C	⇒ C-C-CO-*C + CO-C-C-C-C-C-C + 2 OH	1.00E+11	20500
C-C-COOH-C-C-COO*-C-C-C-C-C	⇒ C-C-CO-C-*C + CO-C-C-C-C-C + 2 OH	4.00E+10	20500
COO*-C-C-COOH-C-C-C-C-C-C	⇒ *C-C-CO-C-C-C-C-C-C + CO + 2 OH	4.00E+10	20500
C-COO*-C-COOH-C-C-C-C-C-C	⇒ *C-C-CO-C-C-C-C-C-C + C-CO + 2 OH	1.00E+11	20500
C-C-COO*-COOH-C-C-C-C-C-C	⇒ *CO-C-C-C-C-C-C-C + C-C-CO + 2 OH	6.30E+11	26600
C-C-C-COOH-COO*-C-C-C-C-C-C	⇒ C-C-C-*CO + CO-C-C-C-C-C-C + 2 OH	6.30E+11	26600
C-C-C-COOH-C-C-COO*-C-C-C-C	⇒ C-C-C-CO-*C + CO-C-C-C-C-C + 2 OH	4.00E+10	20500
C-C-C-C-COOH-C-C-C-C-C-C	⇒ *C-C-CO-C-C-C-C-C-C + C-CO + 2 OH	4.00E+10	20500
C-C-C-C-COOH-C-C-C-C-C-C	⇒ *C-CO-C-C-C-C-C-C-C + C-C-CO + 2 OH	1.00E+11	20500
C-C-C-C-COOH-C-C-C-C-C-C	⇒ C-C-C-C-CO-*C + CO-C-C-C-C-C + 2 OH	6.30E+11	26600
C-C-C-C-COOH-C-C-C-C-C-C	⇒ C-C-C-C-C-CO-*C + C-C-C-CO + 2 OH	6.30E+11	26600
C-C-C-C-C-COOH-C-C-C-C-C	⇒ *C-C-C-C-C-C-C-C + C-C-C-CO + 2 OH	1.00E+11	20500
C-C-C-C-C-COOH-C-C-C-C-C	⇒ C-C-C-C-C-C-C-C + CO-C-C-C-C + 2 OH	4.00E+10	20500
C-C-C-C-C-COOH-C-C-C-C-C	⇒ C-C-C-C-C-C-C-C + CO-C-C-C-C + 2 OH	6.30E+11	26600
C-C-C-C-C-COOH-C-C-C-C-C	⇒ C-C-C-C-C-C-C-C + C-C-C-CO + 2 OH	1.00E+11	20500
C-C-C-C-C-COOH-C-C-C-C-C	⇒ *C-C-C-C-C-C-C-C + C-C-C-CO + 2 OH	4.00E+10	20500
C-C-C-C-C-COOH-C-C-C-C-C	⇒ C-C-C-C-C-C-C-C + CO-C-C-C-C + 2 OH	6.30E+11	26600
C-C-C-C-C-COOH-C-C-C-C-C	⇒ C-C-C-C-C-C-C-C + C-C-C-CO + 2 OH	1.00E+11	20500
C-C-C-C-C-COOH-C-C-C-C-C	⇒ *C-C-C-C-C-C-C-C + C-C-C-CO + 2 OH	4.00E+10	20500
C-C-C-C-C-COOH-C-C-C-C-C	⇒ C-C-C-C-C-C-C-C + CO-C-C-C-C + 2 OH	6.30E+11	26600
C-C-C-C-C-COOH-C-C-C-C-C	⇒ C-C-C-C-C-C-C-C + C-C-C-CO + 2 OH	1.00E+11	20500
C-C-C-C-C-COOH-C-C-C-C-C	⇒ *C-C-C-C-C-C-C-C + C-C-C-CO + 2 OH	4.00E+10	20500

Primary propagation reactions of n-hexadecane oxidation

(Units are kcal, kmole, m, s, K)

Initiation reactions

		A	E
C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C^* + *C-C-C-C-C-C-C-C-C-C-C$	1.00E+17	83000
C-C-C-C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C^* + *C-C-C-C-C-C-C-C-C-C$	1.00E+17	81000
C-C-C-C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C^* + *C-C-C-C-C-C-C-C-C-C$	1.00E+17	81000
C-C-C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C^* + *C-C-C-C-C-C-C-C-C$	1.00E+17	81000
C-C-C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C^* + *C-C-C-C-C-C-C-C$	1.00E+17	81000
C-C-C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-C^* + *C-C-C-C-C-C-C-C$	1.00E+17	81000
C-C-C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-C-C^* + *C-C-C-C-C-C-C-C$	1.00E+17	81000
C-C-C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-C-C-C^* + *C-C-C-C-C-C-C-C$	0.50E+17	81000

H-abstraction reactions

$R^* + C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow *C-C-C-C-C-C-C-C-C-C-C-C-C-C$	6 primary	H atoms
$R^* + C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-*C-C-C-C-C-C-C-C-C-C-C-C-C$	4 secondary	H atoms
$R^* + C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C-*C-C-C-C-C-C-C-C-C-C-C-C$	4 secondary	H atoms
$R^* + C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C-C-*C-C-C-C-C-C-C-C-C-C-C-C$	4 secondary	H atoms
$R^* + C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C-C-C-*C-C-C-C-C-C-C-C-C-C-C$	4 secondary	H atoms
$R^* + C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C-C-C-C-*C-C-C-C-C-C-C-C-C-C$	4 secondary	H atoms
$R^* + C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C-C-C-C-C-*C-C-C-C-C-C-C-C-C$	4 secondary	H atoms
$R^* + C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C-C-C-C-C-C-*C-C-C-C-C-C-C-C$	4 secondary	H atoms

β -decomposition of alkyl radical

$*C-C-C-C-C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C=C + *C-C-C-C-C-C-C-C-C-C$	1.00E+14	30000
$C-*C-C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C=C + *C-C-C-C-C-C-C-C-C-C$	1.00E+14	31000
$C-C-*C-C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C=C-C-C-C-C-C-C-C-C-C-C+C$	1.00E+14	33000
$C-C-*C-C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C-C=C + *C-C-C-C-C-C-C-C-C$	1.00E+14	31000
$C-C-C-*C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C=C-C-C-C-C-C-C-C-C-C+C-*C$	1.00E+14	31000
$C-C-C-*C-C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C-C=C + *C-C-C-C-C-C-C-C-C$	1.00E+14	31000
$C-C-C-C-*C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C=C-C-C-C-C-C-C-C-C+C-C-*C$	1.00E+14	31000
$C-C-C-C-*C-C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C-C-C=C + *C-C-C-C-C-C-C-C$	1.00E+14	31000
$C-C-C-C-C-*C-C-C-C-C-C-C-C-C$	$\Rightarrow C=C-C-C-C-C-C-C-C+C-C-C-*C$	1.00E+14	31000
$C-C-C-C-C-*C-C-C-C-C-C-C-C-C$	$\Rightarrow C-C-C-C=C + *C-C-C-C-C-C-C-C$	1.00E+14	31000
$C-C-C-C-C-C-*C-C-C-C-C-C-C-C$	$\Rightarrow C=C-C-C-C-C-C+C-C-C-C-*C$	1.00E+14	31000
$C-C-C-C-C-C-C-*C-C-C-C-C-C-C$	$\Rightarrow C-C-C-C-C=C + *C-C-C-C-C-C-C$	1.00E+14	31000
$C-C-C-C-C-C-C-C-*C-C-C-C-C-C$	$\Rightarrow C=C-C-C-C-C-C+C-C-C-C-C-*C$	1.00E+14	31000
$C-C-C-C-C-C-C-C-C-*C-C-C-C-C$	$\Rightarrow C-C-C-C-C-C=C + *C-C-C-C-C-C-C$	1.00E+14	31000

Isomerization (H-transfer) of alkyl radical

*C-C-C-C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-^*C-C-C-C-C-C-C-C-C$	1.89E+11	18300
*C-C-C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-^*C-C-C-C-C-C-C-C$	3.00E+10	12200
*C-C-C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	1.20E+10	12200
C-*C-C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-^*C-C-C-C-C-C-C-C$	1.89E+11	19300
C-*C-C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-^*C-C-C-C-C-C-C-C$	3.00E+10	13200
C-*C-C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	1.20E+10	13200
C-*C-C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	1.89E+11	19300
C-C-*C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	3.00E+10	13200
C-C-*C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	1.20E+10	13200
C-C-*C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	1.89E+11	19300
C-C-*C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	3.00E+10	13200
C-C-*C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	1.20E+10	13200
C-C-*C-C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	1.89E+11	21600
C-C-C-*C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	1.89E+11	19300
C-C-C-*C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	3.00E+10	13200
C-C-C-*C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	1.20E+10	13200
C-C-C-*C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	1.89E+11	19300
C-C-C-*C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	4.50E+10	15500
C-C-C-*C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	3.00E+10	13200
C-C-C-*C-C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	1.20E+10	13200
C-C-C-C-*C-C-C-C-C-C-C-C-C-C	$\Rightarrow C-C-C-C-C-^*C-C-C-C-C-C-C$	1.89E+11	19300

O₂ abstractions on of alkyl radicals to form HO₂· and conjugate alkenes

*C-C-C-C-C-C-C-C-C-C-C-C-C + O2	\Rightarrow	C=C-C-C-C-C-C-C-C-C-C-C + HO2	3.00E+08	3500
C-*C-C-C-C-C-C-C-C-C-C-C-C + O2	\Rightarrow	C=C-C-C-C-C-C-C-C-C-C-C + HO2	4.50E+08	3500
C-*C-C-C-C-C-C-C-C-C-C-C-C + O2	\Rightarrow	C-C=C-C-C-C-C-C-C-C-C-C + HO2	3.00E+08	3500
C-C-*C-C-C-C-C-C-C-C-C-C-C + O2	\Rightarrow	C-C=C-C-C-C-C-C-C-C-C-C + HO2	3.00E+08	3500
C-C-*C-C-C-C-C-C-C-C-C-C-C + O2	\Rightarrow	C-C=C-C-C-C-C-C-C-C-C-C + HO2	3.00E+08	3500
C-C-*C-C-C-C-C-C-C-C-C-C-C + O2	\Rightarrow	C-C-C=C-C-C-C-C-C-C-C-C + HO2	3.00E+08	3500
C-C-C-*C-C-C-C-C-C-C-C-C-C + O2	\Rightarrow	C-C-C=C-C-C-C-C-C-C-C-C + HO2	3.00E+08	3500
C-C-C-*C-C-C-C-C-C-C-C-C-C + O2	\Rightarrow	C-C-C=C-C-C-C-C-C-C-C + HO2	3.00E+08	3500
C-C-C-C-*C-C-C-C-C-C-C-C-C + O2	\Rightarrow	C-C-C=C-C-C-C-C-C-C-C + HO2	3.00E+08	3500
C-C-C-C-*C-C-C-C-C-C-C-C-C + O2	\Rightarrow	C-C-C=C-C-C-C-C-C-C + HO2	3.00E+08	3500
C-C-C-C-C-*C-C-C-C-C-C-C-C + O2	\Rightarrow	C-C-C=C-C-C-C-C-C-C + HO2	3.00E+08	3500
C-C-C-C-C-*C-C-C-C-C-C-C-C + O2	\Rightarrow	C-C-C=C-C-C-C-C-C-C + HO2	3.00E+08	3500
C-C-C-C-C-C-*C-C-C-C-C-C-C + O2	\Rightarrow	C-C-C=C-C-C-C-C-C-C + HO2	3.00E+08	3500
C-C-C-C-C-C-*C-C-C-C-C-C-C + O2	\Rightarrow	C-C-C=C-C-C-C-C-C-C + HO2	3.00E+08	3500
C-C-C-C-C-C-C-*C-C-C-C-C-C + O2	\Rightarrow	C-C-C=C-C-C-C-C-C-C + HO2	3.00E+08	3500
C-C-C-C-C-C-C-C-*C-C-C-C-C + O2	\Rightarrow	C-C-C=C-C-C-C-C-C-C + HO2	3.00E+08	3500

O₂ addition on alkyl radicals to form peroxy radicals (and reverse reactions)

C-C-C-C-C-C-C-C-C-C-C-C-C-C-C +O2	⇒ COO-C-C-C-C-C-C-C-C-C-C-C-C-C-C	1.00E+09	0
COO*-C-C-C-C-C-C-C-C-C-C-C-C-C	⇒ *C-C-C-C-C-C-C-C-C-C-C-C-C-C +O2	3.00E+13	30000
C-*C-C-C-C-C-C-C-C-C-C-C-C-C +O2	⇒ C-COO*-C-C-C-C-C-C-C-C-C-C-C-C	1.00E+09	0
C-COO*-C-C-C-C-C-C-C-C-C-C-C-C	⇒ C-*C-C-C-C-C-C-C-C-C-C-C-C-C +O2	3.00E+13	30000
C-C-*C-C-C-C-C-C-C-C-C-C-C-C +O2	⇒ C-C-COO*-C-C-C-C-C-C-C-C-C-C-C	1.00E+09	0
C-C-COO*-C-C-C-C-C-C-C-C-C-C-C	⇒ C-C-*C-C-C-C-C-C-C-C-C-C-C-C +O2	3.00E+13	30000
C-C-C-*C-C-C-C-C-C-C-C-C-C-C +O2	⇒ C-C-C-COO*-C-C-C-C-C-C-C-C-C-C	1.00E+09	0
C-C-C-COO*-C-C-C-C-C-C-C-C-C-C	⇒ C-C-C-*C-C-C-C-C-C-C-C-C-C +O2	3.00E+13	30000
C-C-C-C-*C-C-C-C-C-C-C-C-C-C +O2	⇒ C-C-C-C-COO*-C-C-C-C-C-C-C-C-C	1.00E+09	0
C-C-C-C-COO*-C-C-C-C-C-C-C-C-C	⇒ C-C-C-C-C-*C-C-C-C-C-C-C-C +O2	3.00E+13	30000
C-C-C-C-C-*C-C-C-C-C-C-C-C-C +O2	⇒ C-C-C-C-C-COO*-C-C-C-C-C-C-C-C	1.00E+09	0
C-C-C-C-C-C-COO*-C-C-C-C-C-C-C	⇒ C-C-C-C-C-C-C-*C-C-C-C-C-C +O2	3.00E+13	30000

Isomerization of ROO[·] to QOOH radicals

COO*-C-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	COOH-*C-C-C-C-C-C-C-C-C-C-C-C	1.26E+12	26800
COO*-C-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	COOH-C-*C-C-C-C-C-C-C-C-C-C-C	2.00E+11	20700
COO*-C-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	COOH-C-C-*C-C-C-C-C-C-C-C-C-C	8.00E+10	20700
C-COO*-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	*C-COOH-C-C-C-C-C-C-C-C-C-C-C	1.89E+12	29100
C-COO*-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-COOH-*C-C-C-C-C-C-C-C-C-C-C	1.26E+12	26800
C-COO*-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-COOH-*C-C-C-C-C-C-C-C-C-C-C	2.00E+11	20700
C-COO*-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-COOH-C-C-*C-C-C-C-C-C-C-C-C	8.00E+10	20700
C-C-COO*-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-*C-COOH-C-C-C-C-C-C-C-C-C-C	1.26E+12	26800

Isomerization of 'QOOH to ROO' to radicals

COOH-*C-C-C-C-C-C-C-C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C-C-C-C	9.45E+10	19100
COOH-C-*C-C-C-C-C-C-C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C-C-C-C	1.50E+10	13000
COOH-C-C-*C-C-C-C-C-C-C-C-C-C-C-C	⇒ COO*-C-C-C-C-C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-COOH-C-C-C-C-C-C-C-C-C-C-C-C-C	⇒ C-COO-C-C-C-C-C-C-C-C-C-C-C-C-C	9.45E+10	18100
C-COOH-*C-C-C-C-C-C-C-C-C-C-C-C-C	⇒ C-COO*-C-C-C-C-C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-COOH-C-*C-C-C-C-C-C-C-C-C-C-C-C	⇒ C-COO*-C-C-C-C-C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-COOH-C-C-*C-C-C-C-C-C-C-C-C-C-C	⇒ C-COO*-C-C-C-C-C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-C-COOH-C-C-C-C-C-C-C-C-C-C-C-C	⇒ C-C-COO-C-C-C-C-C-C-C-C-C-C-C-C	1.50E+10	12000
C-*C-COOH-C-C-C-C-C-C-C-C-C-C-C-C	⇒ C-C-COO*-C-C-C-C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-COOH-*C-C-C-C-C-C-C-C-C-C-C-C	⇒ C-C-COO*-C-C-C-C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-COOH-C-*C-C-C-C-C-C-C-C-C-C-C	⇒ C-C-COO*-C-C-C-C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-COOH-C-C-*C-C-C-C-C-C-C-C-C-C	⇒ C-C-COO*-C-C-C-C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-C-C-COOH-C-C-C-C-C-C-C-C-C-C-C	⇒ C-C-C-COO-C-C-C-C-C-C-C-C-C-C-C	6.00E+09	12000
C-*C-C-COOH-C-C-C-C-C-C-C-C-C-C-C	⇒ C-C-C-COO*-C-C-C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-*C-COOH-C-C-C-C-C-C-C-C-C-C-C	⇒ C-C-C-COO*-C-C-C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-C-COOH-*C-C-C-C-C-C-C-C-C-C-C	⇒ C-C-C-COO*-C-C-C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-C-COOH-C-C-*C-C-C-C-C-C-C-C-C	⇒ C-C-C-COO*-C-C-C-C-C-C-C-C-C-C-C	1.50E+10	19100
C-C-C-C-COOH-*C-C-C-C-C-C-C-C-C-C	⇒ C-C-C-C-COO*-C-C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-C-C-C-COOH-C-C-*C-C-C-C-C-C-C-C	⇒ C-C-C-C-COO*-C-C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-C-C-C-COOH-*C-C-C-C-C-C-C-C-C	⇒ C-C-C-C-C-COO*-C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-C-C-C-C-COOH-C-C-*C-C-C-C-C-C	⇒ C-C-C-C-C-C-COO*-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-C-C-C-C-C-COOH-*C-C-C-C-C-C-C	⇒ C-C-C-C-C-C-C-COO*-C-C-C-C-C-C-C	9.45E+10	19100
C-C-C-C-C-C-C-C-COOH-C-C-*C-C-C-C	⇒ C-C-C-C-C-C-C-C-COO*-C-C-C-C-C-C	1.50E+10	13000
C-C-C-C-C-C-C-C-C-C-COOH-*C-C-C-C	⇒ C-C-C-C-C-C-C-C-C-C-COO*-C-C-C-C	6.00E+09	13000
C-C-C-C-C-C-C-C-C-C-C-COOH-C-C-*C	⇒ C-C-C-C-C-C-C-C-C-C-C-COO*-C-C-C	6.00E+09	13000
C-C-C-C-C-C-C-C-C-C-C-C-COOH-*C-C	⇒ C-C-C-C-C-C-C-C-C-C-C-C-COO*-C-C	1.50E+10	13000
C-C-C-C-C-C-C-C-C-C-C-C-C-COOH-C	⇒ C-C-C-C-C-C-C-C-C-C-C-C-C-COOH-C	9.45E+10	19100

C-C-C-C-C-COOH-*C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-C-C-C-COOH-C-*C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-C-C-C-COOH-C-C-*C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-C-C-*C-C-C-C-COOH-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-C-C-C-*C-C-C-C-COOH-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-C-C-C-*C-C-C-C-COOH-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-C-C-C-C-COOH-*C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-C-C-C-C-COOH-C-*C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-C-C-C-C-COOH-C-C-*C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-C-C-C-C-C-COOH-C-C-C-*C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-C-C-C-C-C-COOH-C-C-C-C-*C-C-C-C-C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-C-C-C-C-COOH-C-C-C-C-C-*C-C-C-C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-C-C-C-C-COOH-C-C-C-C-C-C-*C-C-C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	9.45E+10	19100
C-C-C-C-C-C-COOH-C-C-C-C-C-C-C-*C-C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-C-C-C-C-COOH-C-C-C-C-C-C-C-C-*C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-C-C-C-C-C-COOH-C-C-C-C-C-C-C-C-C-*C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	6.00E+09	13000
C-C-C-C-C-C-COOH-C-C-C-C-C-C-C-C-C-C-*	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	1.50E+10	13000
C-C-C-C-C-C-COOH-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-C-COO-*C-C-C-C-C-C-C-C-C	9.45E+10	19100

Decomposition of 'QOOH radicals to form small alkenes and aldehydes

Decomposition of 'QOOH radicals to form HO₂' and conjugate alkenes

COOH-*C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C=C-C-C-C-C-C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
*C-COOH-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C=C-C-C-C-C-C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-COOH-*C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C=C-C-C-C-C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-*C-COOH-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C=C-C-C-C-C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-COOH-*C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C=C-C-C-C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-*C-COOH-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C=C-C-C-C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-COOH-*C-C-C-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C=C-C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-*C-COOH-C-C-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C=C-C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-C-C-COOH-*C-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-C=C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-C-C-C-COOH-*C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-C=C-C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-C-C-C-C-COOH-*C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-C-C=C-C-C-C-C-C-C + HO2	1.00E+14	23000
C-C-C-C-C-C-C-C-COOH-*C-C-C-C-C-C-C-C-C-C	\Rightarrow	C-C-C-C-C-C-C=C-C-C-C-C-C + HO2	1.00E+14	23000

Decomposition of 'OOOH' radicals to form cyclic ethers and OH

COOH-*C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	$\text{^C-}^{\wedge}\text{C-C-C-C-C-C-C-C-C-C-C-C-C-C}$	9.45E+11	18000
COOH-C-*C-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	$\text{^C-C-}^{\wedge}\text{C-C-C-C-C-C-C-C-C-C-C-C-C}$	1.50E+11	17000
COOH-C-C-*C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	$\text{^C-C-C-}^{\wedge}\text{C-C-C-C-C-C-C-C-C-C-C-C}$	2.40E+10	8500
*C-COOH-C-C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	$\text{^C-}^{\wedge}\text{C-C-C-C-C-C-C-C-C-C-C-C-C}$	9.45E+11	18000
C-COOH-*C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	$\text{C-}^{\wedge}\text{C-}^{\wedge}\text{C-C-C-C-C-C-C-C-C-C-C-C}$	9.45E+11	18000
C-COOH-*C-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	$\text{C-}^{\wedge}\text{C-C-}^{\wedge}\text{C-C-C-C-C-C-C-C-C-C-C}$	1.50E+11	17000
C-COOH-C-C-*C-C-C-C-C-C-C-C-C-C	\Rightarrow	$\text{C-}^{\wedge}\text{C-C-C-}^{\wedge}\text{C-C-C-C-C-C-C-C-C-C}$	2.40E+10	8500
*C-C-COOH-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	$\text{^C-C-}^{\wedge}\text{C-C-C-C-C-C-C-C-C-C-C-C}$	1.50E+11	17000
C-*C-COOH-C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	$\text{C-}^{\wedge}\text{C-C-}^{\wedge}\text{C-C-C-C-C-C-C-C-C-C-C}$	9.45E+11	18000
C-C-COOH-*C-C-C-C-C-C-C-C-C-C-C	\Rightarrow	$\text{C-C-}^{\wedge}\text{C-C-}^{\wedge}\text{C-C-C-C-C-C-C-C-C-C}$	9.45E+11	18000
C-C-COOH-C-*C-C-C-C-C-C-C-C-C-C	\Rightarrow	$\text{C-C-}^{\wedge}\text{C-C-}^{\wedge}\text{C-C-C-C-C-C-C-C-C-C}$	1.50E+11	17000
C-C-COOH-C-C-*C-C-C-C-C-C-C-C	\Rightarrow	$\text{C-C-C-}^{\wedge}\text{C-C-C-C-C-C-C-C-C-C-C}$	2.40E+10	8500

O₂ addition on 'QOOH to form 'OOQOOH radicals (and reverse reactions)

Decomposition of 'OOQOOH radicals to form keto-hydroperoxides (OQOOH)

