Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Stochastic methods for aerosol chemistry: a compact molecular description of functionalization and fragmentation in the heterogeneous oxidation of squalane aerosol by OH radicals

A. A. Wiegel,[a] K. R. Wilson,[a] W. D. Hinsberg,[b] and F. A. Houle [a]

[a] Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA.
[b] Columbia Hill Technical Consulting, Fremont, CA 94539, USA.

S-1. Calculating the molecular density

To initialize the calculation, the molecular volume of squalane (i.e. the inverse of density, ρ_{Sq}) is divided equally among the 30 different reactive sites corresponding to the 30 carbon atoms. The molecular volume of each is assigned to the associated hydrogen species within the reactive site by dividing by their number on that carbon (N_H) as in Eq. (1).

$$\rho_{H} = N_{H} N_{C} \rho_{Sq} \qquad (1)$$

For example, using the molecular density of squalane (1.154×10^{21} cm^{-3}), the density of any secondary hydrogen species is 6.922×10^{22} cm^{-3}. Once oxygen functional groups are added to the molecule, the density was assumed to increase by 0.03 g cm^{-3} for each oxygen added weighted by its fraction of the whole particle as in Wilson et al.[1] To find the molecular density of the extra functional group, the molecular volume (i.e. the inverse of the density) of the remaining hydrogens is subtracted from the molecular volume of the functionalized molecule (e.g. squalanone) to give the density of a single functional group using Eq. (2).

$$\frac{1}{\rho_{func}} = \frac{1}{\rho_{SqO}} - \left(\sum \frac{1}{\rho_{H}}\right) \qquad (2)$$

For example, a secondary squalanone isomer ($C_{30}H_{60}O$) has a total molecular volume of 8.635×10^{-22} cm^3 (from a molecular density of 1.158×10^{21} cm^{-3}), and the sum of the molecular volumes of the remaining 6 tertiary hydrogens, 24 primary hydrogens, and 30 secondary hydrogens is 8.379×10^{-22} cm^3. Therefore, the molecular density of the ketone functional group is 3.909×10^{22} cm^{-3}. Using this parameterization of the density, the model adjusts the volume of the whole particle (and thus the concentrations of each species) as functional groups are added. Table S-1 lists the molecular density of each species in the model.

Table S-1 Molecular density of hydrogen sites, functional groups, and carbon fragments

Species	Density (cm^{-3})
tert-H	3.4609×10^{22}
α-H	6.9218×10^{22}
β-H	6.9218×10^{22}
prim-H	1.0383×10^{23}
tert-OH	3.3824×10^{22}
α-OH	6.6147×10^{22}
β-OH	6.6147×10^{22}
α-C=O	3.9093×10^{22}
β-C=O	3.9093×10^{22}
C_3	1.7535×10^{22}
C_4	1.7901×10^{22}
C_5	1.8282×10^{22}
C_6	1.8680×10^{22}
C_8	1.9529×10^{22}
C_9	1.9984×10^{22}
C_{10}	2.0460×10^{22}
C_{11}	2.0960×10^{22}
C_{13}	2.2036×10^{22}
C_{14}	2.2616×10^{22}
C_{15}	2.3228×10^{22}
C_{16}	2.3874×10^{22}
C_{17}	2.4557×10^{22}
C_{19}	2.6047×10^{22}
C_{20}	2.6862×10^{22}
C_{21}	2.7729×10^{22}
C_{22}	2.8655×10^{22}
C_{24}	3.0705×10^{22}
C_{25}	3.1843×10^{22}
C_{26}	3.3070×10^{22}
C_{27}	3.4395×10^{22}
All other species[a]	10^{100}

[a]The density of all other species (e.g. C_{30}) was set at 10^{100} cm^{-3} so that they would not influence the overall volume

Table S-2 Rate coefficients for the hydrogen abstraction by OH and by alkoxy radicals using two different model assumptions based on gas-phase (I)[2] and aqueous (II)[3,4] SAR and for the formation of peroxy radicals.

Reaction	k (I)	k (II)
tert-H → *tert*-R	1.28×10^{-2} s^{-1}	5.82×10^{-3} s^{-1}
α-H → α-R	1.60×10^{-3} s^{-1}	2.91×10^{-3} s^{-1}
β-H → β-R	1.60×10^{-3} s^{-1}	2.91×10^{-3} s^{-1}
α-H-COH → α-RCOH	1.66×10^{-2} s^{-1}	1.00×10^{-2} s^{-1}
β-H-COH → β-RCOH	1.66×10^{-2} s^{-1}	1.00×10^{-2} s^{-1}
(any) RO + *tert*-H → *tert*-R + ROH	1.66×10^{-16} cm^3 s^{-1}	7.55×10^{-17} cm^3 s^{-1}
(any) RO + α-H → α-R + ROH	2.08×10^{-17} cm^3 s^{-1}	3.77×10^{-17} cm^3 s^{-1}
(any) RO + β-H → β-R + ROH	2.08×10^{-17} cm^3 s^{-1}	3.77×10^{-17} cm^3 s^{-1}
(any) RO + α-H-COH → α-RCOH + ROH	4.73×10^{-16} cm^3 s^{-1}	1.29×10^{-16} cm^3 s^{-1}
(any) RO + β-H-COH → β-RCOH + ROH	4.73×10^{-16} cm^3 s^{-1}	1.29×10^{-16} cm^3 s^{-1}
(any) R → ROO	5.54×10^{5} s^{-1}	5.54×10^{5} s^{-1}
α-C(OO)OH → α-C=O	1.00×10^{3} s^{-1}	1.00×10^{3} s^{-1}
β-C(OO)OH → β-C=O	1.00×10^{3} s^{-1}	1.00×10^{3} s^{-1}
p-frag-HCOH → *p-frag*-RCOH[a]	8.28×10^{-3} s^{-1}	5.00×10^{-3} s^{-1}
p-frag-C(=O)H → *p-frag*-RC=O	4.12×10^{-2} s^{-1}	1.89×10^{-2} s^{-1}
s-frag-HCOH → *p-frag*-RCOH	1.66×10^{-2} s^{-1}	1.00×10^{-2} s^{-1}
(any) RO + *p-frag*-HCOH → *p-frag*-RCOH + ROH	5.91×10^{-17} cm^3 s^{-1}	6.5×10^{-17} cm^3 s^{-1}
(any) RO + *p-frag*-C(O)H → *p-frag*-RC=O + ROH	5.34×10^{-16} cm^3 s^{-1}	2.45×10^{-16} cm^3 s^{-1}
(any) RO + *s-frag*-HCOH → *s-frag*-RCOH + ROH	4.73×10^{-16} cm^3 s^{-1}	1.29×10^{-16} cm^3 s^{-1}
p-frag-C(OO)OH → *p-frag*-C(O)H	1.00×10^{3} s^{-1}	1.00×10^{3} s^{-1}

[a] The prefix *p-frag*- refers to primary fragment functional group. The prefix *s-frag*- refers to a secondary fragment functional group.

S-2. Electronic Structure Calculations

To estimate the effect of solvation on the rate coefficient for alkoxy decomposition, electronic structure calculations of the barrier height of the transition state are performed in GAUSSIAN09.[5] Model compounds are chosen based on their structural similarity to squalane-derived alkoxy radicals and to alkoxy radicals from previous measurements[6] and calculations[7] of barrier heights. The geometries are optimized, and the energies are calculated are calculated using B3LYP[8,9] and the 6-31G basis set. Transition states are identified by a single imaginary force constant for a vibration that connects the reactants and the products. Calculations are done both in the gas phase and in the condensed phase using a polarizable continuum model (PCM)[10] of solvation with n-hexadecane as the solvent. The difference in barrier heights calculated for the alkoxy scission is used with the experimental barrier heights to estimate the approximate change in rate coefficient in the condensed phase. Using the value of A_{TST} (1.8×10^{13} s^{-1}) recommended by Peeters et al.,[11] this typical reduction in barrier height increases the rate coefficient for decomposition by a factor of 5. Optimized geometries are included with the text for this supplement.

S-3. Evaporation Rate Coefficient

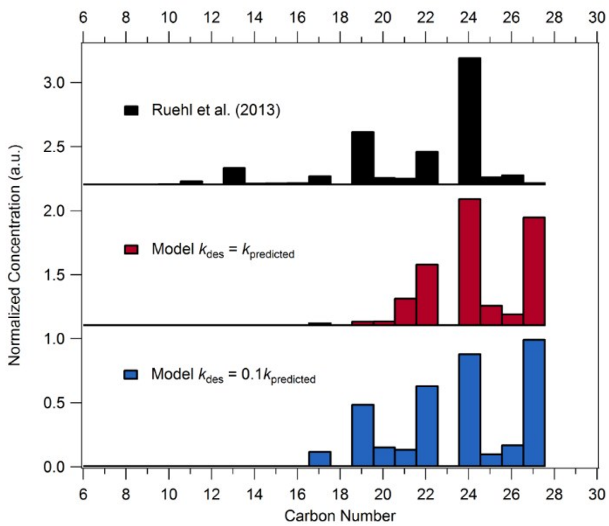

Figure S-1. Comparison of the carbon number distribution of products from Ruehl et al.[12] and two model scenarios. One model scenario directly uses the predicted desorption rate coefficient, while the other scales that value down by a factor of 10. Both the experimental and the model results are normalized to the highest peak in the distribution of carbon number products.

The evaporation rate coefficient is constrained using model assumption "a" and the measured carbon fragment distribution from Ruehl et al.[12] Both the experimental data and the model output were re-normalized to the largest carbon fragment in the distribution to qualitatively compare the two distributions. Because analytical standards of the fragmentation products of squalane are not available, a more quantitative comparison between the model and experimental carbon fragment distribution is not possible. However, since the relative differences in evaporate rate coefficients in the model mostly depend on the carbon number, reducing the rate coefficient by a factor of 10 best approximates the carbon fragment distribution from experiment. (Figure S-1) This reduction in the rate coefficient is consistent with the relative errors for SIMPOL.1 in predicting the vapor pressures of aldehydes, ketones, and alcohols[13] and the likely non-ideal evaporation behavior of mixtures of squalane and its oxidation products, so it is used for each subsequent model scenario involving fragmentation. A list of the predicted vapor pressures and evaporation rate coefficients is given in Table S-3.

Table S-3 The vapor pressures of alcohol, aldehyde, and ketone fragmentation products estimated from SIMPOL.1[13] and their associated evaporation rate coefficients.

Fragmentation Product	p_{vap} (Pa)	k_{evap} (s^{-1})
C_3H_7OH	1.79×10^3	1.23×10^5
C_3H_6O[a]	3.52×10^4	2.46×10^6
C_4H_9OH	652	4.03×10^4
C_4H_8O	4.94×10^3	3.10×10^5
$C_5H_{11}OH$	238	1.35×10^4
$C_5H_{10}O$	1.80×10^3	1.03×10^5
$C_6H_{13}OH$	86.6	4.56×10^3
$C_6H_{12}O$	657	3.50×10^4
$C_8H_{17}OH$	11.5	538
$C_8H_{16}O$[a]	227	1.07×10^4
$C_9H_{19}OH$	4.20	186
$C_9H_{18}O$	31.9	1.42×10^3
$C_{10}H_{21}OH$	1.53	64.9
$C_{10}H_{20}O$	11.6	495
$C_{11}H_{23}OH$	0.559	22.7
$C_{11}H_{22}O$	4.24	173
$C_{13}H_{27}OH$	0.0744	2.8
$C_{13}H_{26}O$[a]	1.47	55.5
$C_{14}H_{29}OH$	0.0271	0.987
$C_{14}H_{28}O$	0.206	7.52
$C_{15}H_{31}OH$	9.90×10^{-3}	0.349
$C_{15}H_{30}O$	0.0751	2.66
$C_{16}H_{33}OH$	3.61×10^{-3}	0.123
$C_{16}H_{32}O$	0.0274	0.941
$C_{17}H_{35}OH$	1.32×10^{-3}	0.0438
$C_{17}H_{34}O$	9.99×10^{-3}	0.333
$C_{19}H_{39}OH$	1.75×10^{-4}	5.53×10^{-3}
$C_{19}H_{38}O$[a]	3.46×10^{-3}	0.109
$C_{20}H_{41}OH$	6.39×10^{-5}	1.97×10^{-3}
$C_{20}H_{40}O$	4.85×10^{-4}	0.0150
$C_{21}H_{43}OH$	2.33×10^{-5}	7.02×10^{-4}
$C_{21}H_{42}O$	1.77×10^{-4}	5.34×10^{-3}
$C_{22}H_{45}OH$	8.51×10^{-6}	2.51×10^{-4}
$C_{22}H_{44}O$	6.45×10^{-5}	1.91×10^{-3}
$C_{24}H_{49}OH$	1.13×10^{-6}	3.20×10^{-5}
$C_{24}H_{48}O$[a]	2.23×10^{-5}	6.33×10^{-4}
$C_{25}H_{51}OH$	4.13×10^{-7}	1.14×10^{-5}
$C_{25}H_{50}O$	3.13×10^{-6}	8.70×10^{-5}
$C_{26}H_{53}OH$	1.51×10^{-7}	4.10×10^{-6}
$C_{26}H_{52}O$	1.14×10^{-6}	3.12×10^{-5}
$C_{27}H_{55}OH$	5.49×10^{-8}	1.47×10^{-6}
$C_{27}H_{54}O$	4.17×10^{-7}	1.12×10^{-5}

[a] Ketone fragmentation product

Supplement References

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Secondary Alkoxy Ground State
[UB3LYP 6-31G;FOpt]
HF = -429.4660031
S2 = 0.752579

[UB3LYP 6-31G;Freq]
HF = -429.4660031
S2 = 0.752579

[Thermochemistry]
Zero-point Correction = 0.267105
Enthalpy Correction = 0.281059
Free Energy Correction = 0.226873

[Geometry]
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H -3.821019 -0.481506 1.273977
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H -3.680262 -1.577850 -0.113521
C -2.510174 0.253311 -0.312487
C -2.573765 1.723205 0.148458
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H -1.788454 2.338331 -0.301716
H -3.538132 2.163163 -0.130000
C -1.199163 -0.448590 0.149538
H -1.214072 -0.486600 1.261729
C 0.119554 0.226184 -0.294614
H 0.100863 1.275659 0.017975
H 0.151346 0.221007 -1.394260
C 1.368358 -0.476363 0.265803
H 1.389218 -0.365356 1.362313
H 1.275884 -1.550255 0.062119
C 2.709350 0.034489 -0.312164
H 2.654659 -0.058016 -1.409343
C 2.971284 1.515589 0.028028
H 3.933063 1.846861 -0.381765
H 2.194541 2.174046 -0.376767
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C 3.874835 -0.847140 0.178700
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O -1.204000 -1.825189 -0.209992

[Frequencies]
34.5653 55.4579 71.7616
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1535.8977	1537.5022	1539.9826
1547.6772	1548.9863	1550.0081
1555.0524	1558.1858	2888.3502
2997.2418	3011.3725	3020.0152
3030.0643	3035.0129	3035.4487
3036.0119	3040.5153	3080.0802
3099.6757	3104.1896	3104.6957
3108.1896	3111.9731	3113.2452
3116.5594	3130.8071	3151.4615

Secondary Alkoxy Transition State

[UB3LYP 6-31G;FTS]

HF = -429.4433377

S2 = 0.768706

[UB3LYP 6-31G;Freq]

HF = -429.4433377

S2 = 0.768706

[Thermochemistry]

Zero-point Correction = 0.263923

Enthalpy Correction = 0.278515

Free Energy Correction = 0.221917

[Geometry]

C -3.890526 -0.480037 -0.002300

H -4.058166 -0.457578 1.081615

H -4.819343 -0.131626 -0.482812

H -3.714166 -1.515699 -0.301020

C -2.736640 0.400445 -0.398297

C -2.661774 1.781571 0.197384

H -2.697087 1.750064 1.293528

H -1.763394 2.325558 -0.108111

H -3.529238 2.379319 -0.129758

C -1.012363 -0.697503 0.343515

H -1.306098 -0.400031 1.367942

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H 2.677557 0.033271 -1.441325

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H 3.857672 1.983867 -0.386464

H 2.102880 2.183343 -0.292200

H 3.014725 1.670197 1.140787

C 4.019591 -0.725718 0.062100

H 3.930351 -1.773254 -0.249065

H 4.926767 -0.312169 -0.394656

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H -2.419328 0.312743 -1.437869

O -1.284424 -1.878013 -0.061341

[Frequencies]

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393.5009 427.0385 437.4151

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840.6993 842.7928 876.2087

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969.1411 973.8508 987.9783

989.9525 1034.2532 1043.9055

1144.8439 1154.5302 1160.9262

1187.9518 1218.1469 1225.0334

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1401.7940	1402.5863	1446.6804
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1501.3431	1518.7141	1519.7813
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1537.1152	1542.0677	1544.7888
1548.8981	1555.1533	2935.3099
2998.1739	3000.9210	3007.3439
3018.0053	3031.6335	3036.5357
3050.5006	3072.8949	3076.7996
3084.3255	3101.2771	3108.5035
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Tertiary Alkoxy Ground State

[UB3LYP 6-31G;FOpt]

HF = -429.4688094

S2 = 0.752339

[UB3LYP 6-31G;Freq]

HF = -429.4688094

S2 = 0.752339

[Thermochemistry]

Zero-point Correction = 0.267151

Enthalpy Correction = 0.281228

Free Energy Correction = 0.226932

[Geometry]

C 3.569797 -0.878026 -0.489608

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[Frequencies]

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250.1617	255.5960	317.9571
342.0189	381.8926	399.8140
404.6793	442.1443	480.3414
526.3040	756.2065	767.6398
827.2848	844.7357	875.3068
939.7766	952.7495	959.1185

967.3097	989.0578	989.2437
1025.6383	1049.9310	1075.6890
1096.9516	1149.3909	1180.1817
1212.2994	1219.5521	1243.8497
1260.1758	1313.7246	1336.7272
1355.8949	1368.8561	1397.0249
1402.0724	1413.7271	1430.1692
1446.2744	1452.0733	1464.2590
1514.0175	1526.9484	1530.1691
1531.3986	1535.3776	1535.9449
1540.1625	1548.2744	1553.1522
1554.4506	1557.8650	2998.2382
3006.2981	3022.5702	3028.6873
3034.7577	3040.7996	3044.7383
3050.1596	3059.2882	3061.1697
3095.8989	3098.3947	3106.2994
3110.8523	3119.6452	3128.2610
3141.5952	3146.6632	3163.7035

Tertiary Alkoxy Transition State

[UB3LYP 6-31G;FTS]

HF = -429.4436293

S2 = 0.770899

[UB3LYP 6-31G;Freq]

HF = -429.4436293

S2 = 0.770899

[Thermochemistry]

Zero-point Correction = 0.263627

Enthalpy Correction = 0.278201

Free Energy Correction = 0.221733

[Geometry]

C 3.686623 -0.935100 -0.345873

H 3.570231 -1.057738 -1.427033

H 4.715127 -0.596120 -0.157414

H 3.553173 -1.898323 0.152427

C 2.718280 0.094628 0.235039

C 2.708470 1.459219 -0.454508

H 2.638217 1.379458 -1.543351

H 1.888078 2.071836 -0.074208

H 3.649816 1.974599 -0.216988

C 0.882300 -0.733652 -0.561832

H 1.051091 -1.745562 -0.198534

H 1.104586 -0.590301 -1.619331

C -0.281784 0.010473 0.027437

H -0.283243 1.048716 -0.325296

H -0.169946 0.039761 1.118458

C -1.639156 -0.656187 -0.330169

H -1.779937 -0.648615 -1.422026

H -1.601607 -1.712512 -0.027201

C -2.867665 0.007050 0.340784

H -2.681673 0.025878 1.426614

C -3.084923 1.458071 -0.132175

H -3.973087 1.892007 0.342555

H -2.233132 2.102656 0.110221

H -3.237355 1.491974 -1.219559

C -4.132626 -0.837891 0.088756

H -4.007585 -1.863252 0.456999

H -5.004343 -0.401957 0.591271

H -4.357400 -0.890619 -0.984992

O 2.402734 0.022306 1.476579

[Frequencies]

-407.6714 19.0303 36.8585

68.2888 94.7665 116.0349

184.5640 195.0679 206.6797

223.2518	226.8060	244.7793
250.9856	317.1809	386.6350
390.2115	430.7496	459.3583
487.2916	502.9267	644.8784
773.3505	779.3038	828.5372
896.1894	932.9704	934.1926
957.6414	968.1131	988.5467
992.1336	1023.4977	1053.8020
1078.2481	1088.8322	1107.5696
1163.7637	1214.0690	1231.3597
1237.8244	1301.4500	1322.3420
1346.0594	1375.3616	1392.9287
1402.7094	1432.8444	1435.7256
1446.5431	1461.9573	1463.7396
1500.3696	1518.1635	1522.0032
1526.6018	1533.7465	1536.0699
1540.1441	1546.4332	1547.0831
1549.3166	1554.5534	3006.2328
3016.4059	3030.2622	3036.3819
3037.5520	3042.6889	3052.0351
3056.9715	3100.0870	3102.1274
3108.3849	3111.5603	3113.0853
3116.9581	3121.9323	3125.1360
3158.3963	3163.3907	3226.6745

Example Reaction Scheme

Time Units: sec

Temperature Units: °K

Energy Units: kJ

Concentration Units: molecules/cm³

Pressure Units: torr

Length Units: m

Temperature Option: Constant Temperature

Pressure Option: Constant Pressure

Volume Option: Variable Volume

Temperature: 298.15

This Compartment Contains the Following Reaction Steps:

Equation: H_sec => R_sec + H2O

Forward k: 2.91E-3

This Reaction uses a Standard Rate Law

Equation: H_sec_a => R_sec_a + H2O

Forward k: 2.91E-3

This Reaction uses a Standard Rate Law

Equation: H_sec_b => R_sec_b + H2O

Forward k: 2.91E-3

This Reaction uses a Standard Rate Law

Equation: H_beta => R_beta + H2O

Forward k: 2.91E-3

This Reaction uses a Standard Rate Law

Equation: H_beta_a => R_beta_a + H2O

Forward k: 2.91E-3

This Reaction uses a Standard Rate Law

Equation: H_tert => R_tert + H2O

Forward k: 5.82E-3

This Reaction uses a Standard Rate Law

Equation: H_tert_a => R_tert_a + H2O

Forward k: 5.82E-3

This Reaction uses a Standard Rate Law

Equation: OH_sec + H_sec_alc => R_OH_sec + H2O

Forward k: 1E-2

This Reaction uses a Nonstandard Rate Law

Equation: OH_beta + H_beta_alc => R_OH_beta + H2O

Forward k: 1E-2

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f + H_prim_f => R_OH_prim_f + H2O

Forward k: 5E-3

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f + H_prim_f => R_OC_prim_f + H2O + aldehyde_abs

Forward k: 1.89E-2

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f2 + H_prim_f2 => R_OH_prim_f2 + H2O

Forward k: 5E-3

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f2 + H_prim_f2 => R_OC_prim_f2 + H2O + aldehyde_abs

Forward k: 1.89E-2

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f3 + H_prim_f3 => R_OH_prim_f3 + H2O

Forward k: 5E-3

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f3 + H_prim_f3 => R_OC_prim_f3 + H2O + aldehyde_abs

Forward k: 1.89E-2

This Reaction uses a Nonstandard Rate Law

Equation: R_sec + H_tert + 2 H_beta => OO_sec + H_tert_a + 2 H_beta_a

Forward k: 5.54E5

This Reaction uses a Nonstandard Rate Law

Equation: R_sec_a => OO_sec_a

Forward k: 5.54E5

This Reaction uses a Standard Rate Law

Equation: R_sec_b => OO_sec_b

Forward k: 5.54E5

This Reaction uses a Standard Rate Law

Equation: R_beta + 4 H_sec => OO_beta + 4 H_sec_b

Forward k: 3.69E5

This Reaction uses a Nonstandard Rate Law

Equation: R_beta + 2 H_sec + 2 H_beta => OO_beta + 4 H_sec_b

Forward k: 1.86E5

This Reaction uses a Nonstandard Rate Law

Equation: R_beta_a => OO_beta_a

Forward k: 5.54E5

This Reaction uses a Standard Rate Law

Equation: R_tert + 2 H_sec => OO_tert + 2 H_sec_a

Forward k: 1.85E5

This Reaction uses a Nonstandard Rate Law

Equation: R_tert + 4 H_sec => OO_tert + 4 H_sec_a

Forward k: 3.69E5

This Reaction uses a Nonstandard Rate Law

Equation: R_tert_a => OO_tert_a

Forward k: 5.54E5

This Reaction uses a Standard Rate Law

Equation: R_sec_f => OO_sec_f

Forward k: 5.54E5

This Reaction uses a Standard Rate Law

Equation: R_prim_f => OO_prim_f

Forward k: 5.54E5

This Reaction uses a Standard Rate Law

Equation: R_prim_f2 => OO_prim_f2

Forward k: 5.54E5

This Reaction uses a Standard Rate Law

Equation: R_prim_f3 => OO_prim_f3

Forward k: 5.54E5

This Reaction uses a Standard Rate Law

Equation: R_prim_f4 => OO_prim_f4

Forward k: 5.54E5

This Reaction uses a Standard Rate Law

Equation: R_OH_sec => OO_OH_sec

Forward k: 1.44E6

This Reaction uses a Standard Rate Law

Equation: R_OH_sec_f => OO_OH_sec_f

Forward k: 1.44E6

This Reaction uses a Standard Rate Law

Equation: R_OH_beta => OO_OH_beta

Forward k: 1.44E6

This Reaction uses a Standard Rate Law

Equation: R_OH_prim_f => OO_OH_prim_f

Forward k: 1.44E6

This Reaction uses a Standard Rate Law

Equation: R_OH_prim_f2 => OO_OH_prim_f2

Forward k: 1.44E6

This Reaction uses a Standard Rate Law

Equation: R_OH_prim_f3 => OO_OH_prim_f3

Forward k: 1.44E6

This Reaction uses a Standard Rate Law

Equation: R_OH_prim_f4 => OO_OH_prim_f4

Forward k: 1.44E6

This Reaction uses a Standard Rate Law

Equation: R_OC_prim_f => OO_OC_prim_f + activate + acyloxy

Forward k: 1.44E6

This Reaction uses a Standard Rate Law

Equation: R_OC_prim_f2 => OO_OC_prim_f2 + activate2 + acyloxy

Forward k: 1.44E6

This Reaction uses a Standard Rate Law

Equation: R_OC_prim_f3 => OO_OC_prim_f3 + activate3 + acyloxy

Forward k: 1.44E6

This Reaction uses a Standard Rate Law

Equation: R_OC_prim_f4 => OO_OC_prim_f4 + activate4 + acyloxy

Forward k: 1.44E6

This Reaction uses a Standard Rate Law

Equation: OO_OH_sec => OC_sec + HO2

Forward k: 1000

This Reaction uses a Standard Rate Law

Equation: OO_OH_sec_f => OC_sec_f + HO2

Forward k: 1000

This Reaction uses a Standard Rate Law

Equation: OO_OH_beta => OC_beta + HO2

Forward k: 1000

This Reaction uses a Standard Rate Law

Equation: OO_OH_prim_f => OC_prim_f + HO2

Forward k: 1000

This Reaction uses a Standard Rate Law

Equation: OO_OH_prim_f2 => OC_prim_f2 + HO2

Forward k: 1000

This Reaction uses a Standard Rate Law

Equation: OO_OH_prim_f3 => OC_prim_f3 + HO2

Forward k: 1000

This Reaction uses a Standard Rate Law

Equation: OO_OH_prim_f4 => OC_prim_f4 + HO2

Forward k: 1000

This Reaction uses a Standard Rate Law

Equation: ROO => ROO

Forward k: 1.0

This Reaction uses a Standard Rate Law

Equation: 2 OO_tert => 2 O_tert + O2 + 2 alkoxy

Forward k: 3.75E-16

This Reaction uses a Standard Rate Law

Equation: 2 OO_tert_a => 2 O_tert_a + O2 + 2 alkoxy_a

Forward k: 3.75E-16

This Reaction uses a Standard Rate Law

Equation: 2 OO_sec + 2 H_sec => 2 OC_sec + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_sec => 2 O_sec + O2 + 2 alkoxy_s

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_sec_a + 2 H_sec_a => 2 OC_sec_a + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_sec_a => 2 O_sec_a + O2 + 2 alkoxy_as

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_sec_b + 2 H_sec_b => 2 OC_sec_b + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_sec_b => 2 O_sec_b + O2 + 2 alkoxy_as

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_beta + 2 H_beta => 2 OC_beta + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_beta => 2 O_beta + O2 + 2 alkoxy_s

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_beta_a + 2 H_beta_a => 2 OC_beta_a + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_beta_a => 2 O_beta_a + O2 + 2 alkoxy_as

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_sec_f + 2 H_sec_f => 2 OC_sec_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_sec_f => 2 O_sec_f + O2 + 2 alkoxy_s

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_prim_f + 2 H_prim_f => 2 OC_prim_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_prim_f => 2 O_prim_f + O2 + 2 alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_prim_f2 + 2 H_prim_f2 => 2 OC_prim_f2 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_prim_f2 => 2 O_prim_f2 + O2 + 2 alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_prim_f3 + 2 H_prim_f3 => 2 OC_prim_f3 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_prim_f3 => 2 O_prim_f3 + O2 + 2 alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_prim_f4 + 2 H_prim_f4 => 2 OC_prim_f4 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: 2 OO_prim_f4 => 2 O_prim_f4 + O2 + 2 alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_tert + H_sec => OC_sec + OH_tert + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_tert => O_sec + O_tert + O2 + alkoxy_s + alkoxy

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_tert + H_sec_a => OC_sec_a + OH_tert + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_tert => O_sec_a + O_tert + O2 + alkoxy_as + alkoxy

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_tert + H_sec_b => OC_sec_b + OH_tert + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_tert => O_sec_b + O_tert + O2 + alkoxy_as + alkoxy

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_tert + H_beta => OC_beta + OH_tert + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_tert => O_beta + O_tert + O2 + alkoxy_s + alkoxy

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta_a + OO_tert + H_beta_a => OC_beta_a + OH_tert + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta_a + OO_tert => O_beta_a + O_tert + O2 + alkoxy_as + alkoxy

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f + OO_tert + H_prim_f => OC_prim_f + OH_tert + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f + OO_tert => O_prim_f + O_tert + O2 + alkoxy_p + alkoxy

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f2 + OO_tert + H_prim_f2 => OC_prim_f2 + OH_tert + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f2 + OO_tert => O_prim_f2 + O_tert + O2 + alkoxy_p + alkoxy

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f3 + OO_tert + H_prim_f3 => OC_prim_f3 + OH_tert + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f3 + OO_tert => O_prim_f3 + O_tert + O2 + alkoxy_p + alkoxy

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f4 + OO_tert + H_prim_f4 => OC_prim_f4 + OH_tert + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f4 + OO_tert => O_prim_f4 + O_tert + O2 + alkoxy_p + alkoxy

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_f + OO_tert + H_sec_f => OC_sec_f + OH_tert + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_f + OO_tert => O_sec_f + O_tert + O2 + alkoxy_fs + alkoxy

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_tert + OO_tert_a => O_tert + O_tert_a + O2 + alkoxy + alkoxy_a

Forward k: 3.75E-16

This Reaction uses a Standard Rate Law

Equation: OO_sec + OO_tert_a + H_sec => OC_sec + OH_tert_a + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_tert_a => O_sec + O_tert_a + O2 + alkoxy_s + alkoxy_a

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_tert_a + H_sec_a => OC_sec_a + OH_tert_a + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_tert_a => O_sec_a + O_tert_a + O2 + alkoxy_as + alkoxy_a

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_tert_a + H_sec_b => OC_sec_b + OH_tert_a + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_tert_a => O_sec_b + O_tert_a + O2 + alkoxy_as + alkoxy_a

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_tert_a + H_beta => OC_beta + OH_tert_a + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_tert_a => O_beta + O_tert_a + O2 + alkoxy_s + alkoxy_a

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta_a + OO_tert_a + H_beta_a => OC_beta_a + OH_tert_a + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta_a + OO_tert_a => O_beta_a + O_tert_a + O2 + alkoxy_as + alkoxy_a

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f + OO_tert_a + H_prim_f => OC_prim_f + OH_tert_a + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f + OO_tert_a => O_prim_f + O_tert_a + O2 + alkoxy_p + alkoxy_a

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f2 + OO_tert_a + H_prim_f2 => OC_prim_f2 + OH_tert_a + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f2 + OO_tert_a => O_prim_f2 + O_tert_a + O2 + alkoxy_p + alkoxy_a

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f3 + OO_tert_a + H_prim_f3 => OC_prim_f3 + OH_tert_a + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f3 + OO_tert_a => O_prim_f3 + O_tert_a + O2 + alkoxy_p + alkoxy_a

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f4 + OO_tert_a + H_prim_f4 => OC_prim_f4 + OH_tert_a + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f4 + OO_tert_a => O_prim_f4 + O_tert_a + O2 + alkoxy_p + alkoxy

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_f + OO_tert_a + H_sec_f => OC_sec_f + OH_tert_a + O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_f + OO_tert_a => O_sec_f + O_tert_a + O2 + alkoxy_fs + alkoxy_a

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_sec_a + H_sec + H_sec_a => OC_sec + OC_sec_a + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_sec_a => O_sec + O_sec_a + O2 + alkoxy_s + alkoxy_as

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_sec_b + H_sec + H_sec_b => OC_sec + OC_sec_b + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_sec_b => O_sec + O_sec_b + O2 + alkoxy_s + alkoxy_as

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_beta + H_sec + H_beta => OC_sec + OC_beta + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_beta => O_sec + O_beta + O2 + 2 alkoxy_s

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_beta_a + H_sec + H_beta_a => OC_sec + OC_beta_a + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_beta_a => O_sec + O_beta_a + O2 + alkoxy_s + alkoxy_as

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_prim_f + H_sec + H_prim_f => OC_sec + OC_prim_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_prim_f => O_sec + O_prim_f + O2 + alkoxy_s + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_prim_f2 + H_sec + H_prim_f2 => OC_sec + OC_prim_f2 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_prim_f2 => O_sec + O_prim_f2 + O2 + alkoxy_s + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_prim_f3 + H_sec + H_prim_f3 => OC_sec + OC_prim_f3 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_prim_f3 => O_sec + O_prim_f3 + O2 + alkoxy_s + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_prim_f4 + H_sec + H_prim_f4 => OC_sec + OC_prim_f4 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_prim_f4 => O_sec + O_prim_f4 + O2 + alkoxy_s + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_sec_f + H_sec + H_sec_f => OC_sec + OC_sec_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec + OO_sec_f => O_sec + O_sec_f + O2 + alkoxy_s + alkoxy_fs

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_sec_b + H_sec_a + H_sec_b => OC_sec_a + OC_sec_b + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_sec_b => O_sec_a + O_sec_b + O2 + alkoxy_s + alkoxy_as

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_beta + H_sec_a + H_beta => OC_sec_a + OC_beta + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_beta => O_sec_a + O_beta + O2 + alkoxy_s + alkoxy_as

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_beta_a + H_sec_a + H_beta_a => OC_sec_a + OC_beta_a + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_beta_a => O_sec_a + O_beta_a + O2 + 2 alkoxy_as

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_prim_f + H_sec_a + H_prim_f => OC_sec_a + OC_prim_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_prim_f => O_sec_a + O_prim_f + O2 + alkoxy_as + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_prim_f2 + H_sec_a + H_prim_f2 => OC_sec_a + OC_prim_f2 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_prim_f2 => O_sec_a + O_prim_f2 + O2 + alkoxy_as + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_prim_f3 + H_sec_a + H_prim_f3 => OC_sec_a + OC_prim_f3 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_prim_f3 => O_sec_a + O_prim_f3 + O2 + alkoxy_as + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_prim_f4 + H_sec_a + H_prim_f4 => OC_sec_a + OC_prim_f4 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_prim_f4 => O_sec_a + O_prim_f4 + O2 + alkoxy_as + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_sec_f + H_sec_a + H_sec_f => OC_sec_a + OC_sec_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_a + OO_sec_f => O_sec_a + O_sec_f + O2 + alkoxy_as + alkoxy_fs

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_beta + H_sec_b + H_beta => OC_sec_b + OC_beta + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_beta => O_sec_b + O_beta + O2 + alkoxy_s + alkoxy_as

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_beta_a + H_sec_b + H_beta_a => OC_sec_b + OC_beta_a + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_beta_a => O_sec_b + O_beta_a + O2 + 2 alkoxy_as

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_prim_f + H_sec_b + H_prim_f => OC_sec_b + OC_prim_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_prim_f => O_sec_b + O_prim_f + O2 + alkoxy_as + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_prim_f2 + H_sec_b + H_prim_f2 => OC_sec_b + OC_prim_f2 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_prim_f2 => O_sec_b + O_prim_f2 + O2 + alkoxy_as + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_prim_f3 + H_sec_b + H_prim_f3 => OC_sec_b + OC_prim_f3 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_prim_f3 => O_sec_b + O_prim_f3 + O2 + alkoxy_as + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_prim_f4 + H_sec_b + H_prim_f4 => OC_sec_a + OC_prim_f4 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_prim_f4 => O_sec_b + O_prim_f4 + O2 + alkoxy_as + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_sec_f + H_sec_b + H_sec_f => OC_sec_b + OC_sec_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_sec_b + OO_sec_f => O_sec_b + O_sec_f + O2 + alkoxy_as + alkoxy_fs

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_beta_a + H_beta + H_beta_a => OC_beta + OC_beta_a + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_beta_a => O_beta + O_beta_a + O2 + alkoxy_s + alkoxy_as

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_prim_f + H_beta + H_prim_f => OC_beta + OC_prim_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_prim_f => O_beta + O_prim_f + O2 + alkoxy_s + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_prim_f2 + H_beta + H_prim_f2 => OC_beta + OC_prim_f2 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_prim_f2 => O_beta + O_prim_f2 + O2 + alkoxy_s + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_prim_f3 + H_beta + H_prim_f3 => OC_beta + OC_prim_f3 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_prim_f3 => O_beta + O_prim_f3 + O2 + alkoxy_s + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_prim_f4 + H_beta + H_prim_f4 => OC_beta + OC_prim_f4 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_prim_f4 => O_beta + O_prim_f4 + O2 + alkoxy_s + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_sec_f + H_beta + H_sec_f => OC_beta + OC_sec_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta + OO_sec_f => O_beta + O_sec_f + O2 + alkoxy_s + alkoxy_fs

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta_a + OO_prim_f + H_beta_a + H_prim_f => OC_beta_a + OC_prim_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta_a + OO_prim_f => O_beta_a + O_prim_f + O2 + alkoxy_as + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta_a + OO_prim_f2 + H_beta_a + H_prim_f2 => OC_beta_a + OC_prim_f2 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta_a + OO_prim_f2 => O_beta_a + O_prim_f2 + O2 + alkoxy_as + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta_a + OO_prim_f3 + H_beta_a + H_prim_f3 => OC_beta_a + OC_prim_f3 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta_a + OO_prim_f3 => O_beta_a + O_prim_f3 + O2 + alkoxy_as + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta_a + OO_prim_f4 + H_beta_a + H_prim_f4 => OC_beta_a + OC_prim_f4 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta_a + OO_prim_f4 => O_beta_a + O_prim_f4 + O2 + alkoxy_as + alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta_a + OO_sec_f + H_beta_a + H_sec_f => OC_beta_a + OC_sec_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_beta_a + OO_sec_f => O_beta_a + O_sec_f + O2 + alkoxy_as + alkoxy_fs

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f + OO_prim_f2 + H_prim_f + H_prim_f2 => OC_prim_f + OC_prim_f2 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f + OO_prim_f2 => O_prim_f + O_prim_f2 + O2 + 2 alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f + OO_prim_f3 + H_prim_f + H_prim_f3 => OC_prim_f + OC_prim_f3 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f + OO_prim_f3 => O_prim_f + O_prim_f3 + O2 + 2 alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f + OO_prim_f4 + H_prim_f + H_prim_f4 => OC_prim_f + OC_prim_f4 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f + OO_prim_f4 => O_prim_f + O_prim_f4 + O2 + 2 alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f + OO_sec_f + H_prim_f + H_sec_f => OC_prim_f + OC_sec_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f + OO_sec_f => O_prim_f + O_sec_f + O2 + alkoxy_p + alkoxy_fs

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f2 + OO_prim_f3 + H_prim_f2 + H_prim_f3 => OC_prim_f2 + OC_prim_f3 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f2 + OO_prim_f3 => O_prim_f2 + O_prim_f3 + O2 + 2 alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f2 + OO_prim_f4 + H_prim_f2 + H_prim_f4 => OC_prim_f2 + OC_prim_f4 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f2 + OO_prim_f4 => O_prim_f2 + O_prim_f4 + O2 + 2 alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f2 + OO_sec_f + H_prim_f2 + H_sec_f => OC_prim_f2 + OC_sec_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f2 + OO_sec_f => O_prim_f2 + O_sec_f + O2 + alkoxy_p + alkoxy_fs

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f3 + OO_prim_f4 + H_prim_f3 + H_prim_f4 => OC_prim_f3 + OC_prim_f4 + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f3 + OO_prim_f4 => O_prim_f3 + O_prim_f4 + O2 + 2 alkoxy_p

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f3 + OO_sec_f + H_prim_f3 + H_sec_f => OC_prim_f3 + OC_sec_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f3 + OO_sec_f => O_prim_f3 + O_sec_f + O2 + alkoxy_p + alkoxy_fs

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f4 + OO_sec_f + H_prim_f4 + H_sec_f => OC_prim_f4 + OC_sec_f + H2O2

Forward k: 1.45E-15

This Reaction uses a Nonstandard Rate Law

Equation: OO_prim_f4 + OO_sec_f => O_prim_f4 + O_sec_f + O2 + alkoxy_p + alkoxy_fs

Forward k: 1.61E-16

This Reaction uses a Nonstandard Rate Law

Equation: ROC_OO => ROC_OO

Forward k: 1.0

This Reaction uses a Standard Rate Law

Equation: 2 OO_OC_prim_f => 2 O_OC_prim_f + O2

Forward k: 5.6E-15

This Reaction uses a Standard Rate Law

Equation: 2 OO_OC_prim_f2 => 2 O_OC_prim_f2 + O2

Forward k: 5.6E-15

This Reaction uses a Standard Rate Law

Equation: 2 OO_OC_prim_f3 => 2 O_OC_prim_f3 + O2

Forward k: 5.6E-15

This Reaction uses a Standard Rate Law

Equation: 2 OO_OC_prim_f4 => 2 O_OC_prim_f4 + O2

Forward k: 5.6E-15

This Reaction uses a Standard Rate Law

Equation: OO_OC_prim_f + OO_OC_prim_f2 => O_OC_prim_f + O_OC_prim_f2 + O2

Forward k: 5.6E-15

This Reaction uses a Standard Rate Law

Equation: OO_OC_prim_f + OO_OC_prim_f3 => O_OC_prim_f + O_OC_prim_f3 + O2

Forward k: 5.6E-15

This Reaction uses a Standard Rate Law

Equation: OO_OC_prim_f + OO_OC_prim_f4 => O_OC_prim_f + O_OC_prim_f4 + O2

Forward k: 5.6E-15

This Reaction uses a Standard Rate Law

Equation: OO_OC_prim_f2 + OO_OC_prim_f3 => O_OC_prim_f2 + O_OC_prim_f3 + O2

Forward k: 5.6E-15

This Reaction uses a Standard Rate Law

Equation: OO_OC_prim_f2 + OO_OC_prim_f4 => O_OC_prim_f2 + O_OC_prim_f4 + O2

Forward k: 5.6E-15

This Reaction uses a Standard Rate Law

Equation: OO_OC_prim_f3 + OO_OC_prim_f4 => O_OC_prim_f3 + O_OC_prim_f4 + O2

Forward k: 5.6E-15

This Reaction uses a Standard Rate Law

Equation: OO_OC_prim_f + OO_tert => O_OC_prim_f + O_tert + O2 + alkoxy

Forward k: 3.75E-16

This Reaction uses a Standard Rate Law

Equation: OO_OC_prim_f2 + OO_tert => O_OC_prim_f2 + O_tert + O2 + alkoxy

Forward k: 3.75E-16

This Reaction uses a Standard Rate Law

Equation: OO_OC_prim_f3 + OO_tert => O_OC_prim_f3 + O_tert + O2 + alkoxy

Forward k: 3.75E-16

This Reaction uses a Standard Rate Law

Equation: OO_OC_prim_f4 + OO_tert => O_OC_prim_f4 + O_tert + O2 + alkoxy

Forward k: 3.75E-16

This Reaction uses a Standard Rate Law

Equation: OO_OC_prim_f + OO_tert_a => O_OC_prim_f + O_tert_a + O2 + alkoxy_a

Forward k: 3.75E-16

This Reaction uses a Standard Rate Law

Equation: OO_OC_prim_f2 + OO_tert_a => O_OC_prim_f2 + O_tert_a + O2 + alkoxy_a

Forward k: 3.75E-16

This Reaction uses a Standard Rate Law

Equation: OO_OC_prim_f3 + OO_tert_a => O_OC_prim_f3 + O_tert_a + O2 + alkoxy_a

Forward k: 3.75E-16

This Reaction uses a Standard Rate Law

Equation: OO_OC_prim_f4 + OO_tert_a => O_OC_prim_f4 + O_tert_a + O2 + alkoxy_a

Forward k: 3.75E-16

This Reaction uses a Standard Rate Law

Equation: OO_OC_prim_f + OO_sec + H_sec => O_OC_prim_f + OC_sec + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_sec => O_OC_prim_f + O_sec + O2 + alkoxy_s

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_sec + H_sec => O_OC_prim_f2 + OC_sec + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_sec => O_OC_prim_f2 + O_sec + O2 + alkoxy_s

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_sec + H_sec => O_OC_prim_f3 + OC_sec + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_sec => O_OC_prim_f3 + O_sec + O2 + alkoxy_s

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_sec + H_sec => O_OC_prim_f4 + OC_sec + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_sec => O_OC_prim_f4 + O_sec + O2 + alkoxy_s

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_sec_a + H_sec_a => O_OC_prim_f + OC_sec_a + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_sec_a => O_OC_prim_f + O_sec_a + O2 + alkoxy_as

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_sec_a + H_sec_a => O_OC_prim_f2 + OC_sec_a + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_sec_a => O_OC_prim_f2 + O_sec_a + O2 + alkoxy_as

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_sec_a + H_sec_a => O_OC_prim_f3 + OC_sec_a + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_sec_a => O_OC_prim_f3 + O_sec_a + O2 + alkoxy_as

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_sec_a + H_sec => O_OC_prim_f4 + OC_sec_a + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_sec_a => O_OC_prim_f4 + O_sec_a + O2 + alkoxy_as

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_sec_b + H_sec_b => O_OC_prim_f + OC_sec_b + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_sec_b => O_OC_prim_f + O_sec_b + O2 + alkoxy_as

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_sec_b + H_sec_b => O_OC_prim_f2 + OC_sec_b + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_sec_b => O_OC_prim_f2 + O_sec_b + O2 + alkoxy_as

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_sec_b + H_sec_b => O_OC_prim_f3 + OC_sec_b + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_sec_b => O_OC_prim_f3 + O_sec_b + O2 + alkoxy_as

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_sec_b + H_sec_b => O_OC_prim_f4 + OC_sec_b + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_sec_b => O_OC_prim_f4 + O_sec_b + O2 + alkoxy_as

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_beta + H_beta => O_OC_prim_f + OC_beta + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_beta => O_OC_prim_f + O_beta + O2 + alkoxy_s

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_beta + H_beta => O_OC_prim_f2 + OC_beta + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_beta => O_OC_prim_f2 + O_beta + O2 + alkoxy_s

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_beta + H_beta => O_OC_prim_f3 + OC_beta + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_beta => O_OC_prim_f3 + O_beta + O2 + alkoxy_s

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_beta + H_beta => O_OC_prim_f4 + OC_beta + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_beta => O_OC_prim_f4 + O_beta + O2 + alkoxy_s

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_beta_a + H_beta_a => O_OC_prim_f + OC_beta_a + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_beta_a => O_OC_prim_f + O_beta_a + O2 + alkoxy_as

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_beta_a + H_beta_a => O_OC_prim_f2 + OC_beta_a + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_beta_a => O_OC_prim_f2 + O_beta_a + O2 + alkoxy_as

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_beta_a + H_beta_a => O_OC_prim_f3 + OC_beta_a + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_beta_a => O_OC_prim_f3 + O_beta_a + O2 + alkoxy_as

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_beta_a + H_beta_a => O_OC_prim_f4 + OC_beta_a + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_beta_a => O_OC_prim_f4 + O_beta_a + O2 + alkoxy_as

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_prim_f + H_prim_f => O_OC_prim_f + OC_prim_f + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_prim_f => O_OC_prim_f + O_prim_f + O2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_prim_f + H_prim_f => O_OC_prim_f2 + OC_prim_f + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_prim_f => O_OC_prim_f2 + O_prim_f + O2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_prim_f + H_prim_f => O_OC_prim_f3 + OC_prim_f + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_prim_f => O_OC_prim_f3 + O_prim_f + O2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_prim_f + H_prim_f => O_OC_prim_f4 + OC_prim_f + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_prim_f => O_OC_prim_f4 + O_prim_f + O2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_prim_f2 + H_prim_f2 => O_OC_prim_f + OC_prim_f2 + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_prim_f2 => O_OC_prim_f + O_prim_f2 + O2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_prim_f2 + H_prim_f2 => O_OC_prim_f2 + OC_prim_f2 + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_prim_f2 => O_OC_prim_f2 + O_prim_f2 + O2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_prim_f2 + H_prim_f2 => O_OC_prim_f3 + OC_prim_f2 + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_prim_f2 => O_OC_prim_f3 + O_prim_f2 + O2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_prim_f2 + H_prim_f2 => O_OC_prim_f4 + OC_prim_f2 + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_prim_f2 => O_OC_prim_f4 + O_prim_f2 + O2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_prim_f3 + H_prim_f3 => O_OC_prim_f + OC_prim_f3 + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_prim_f3 => O_OC_prim_f + O_prim_f3 + O2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_prim_f3 + H_prim_f3 => O_OC_prim_f2 + OC_prim_f3 + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_prim_f3 => O_OC_prim_f2 + O_prim_f3 + O2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_prim_f3 + H_prim_f3 => O_OC_prim_f3 + OC_prim_f3 + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_prim_f3 => O_OC_prim_f3 + O_prim_f3 + HO2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_prim_f3 + H_prim_f3 => O_OC_prim_f4 + OC_prim_f3 + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_prim_f3 => O_OC_prim_f4 + O_prim_f3 + HO2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_prim_f4 + H_prim_f4 => O_OC_prim_f + OC_prim_f4 + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_prim_f4 => O_OC_prim_f + O_prim_f4 + O2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_prim_f4 + H_prim_f4 => O_OC_prim_f2 + OC_prim_f4 + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_prim_f4 => O_OC_prim_f2 + O_prim_f4 + O2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_prim_f4 + H_prim_f4 => O_OC_prim_f3 + OC_prim_f4 + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_prim_f4 => O_OC_prim_f3 + O_prim_f4 + O2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_prim_f4 + H_prim_f4 => O_OC_prim_f4 + OC_prim_f4 + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_prim_f4 => O_OC_prim_f4 + O_prim_f4 + O2 + alkoxy_p

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_sec_f + H_sec_f => O_OC_prim_f + OC_sec_f + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f + OO_sec_f => O_OC_prim_f + O_sec_f + O2 + alkoxy_fs

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_sec_f + H_sec_f => O_OC_prim_f2 + OC_sec_f + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f2 + OO_sec_f => O_OC_prim_f2 + O_sec_f + O2 + alkoxy_fs

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_sec_f + H_sec_f => O_OC_prim_f3 + OC_sec_f + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f3 + OO_sec_f => O_OC_prim_f3 + O_sec_f + O2 + alkoxy_fs

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_sec_f + H_sec_f => O_OC_prim_f4 + OC_sec_f + HO2

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: OO_OC_prim_f4 + OO_sec_f => O_OC_prim_f4 + O_sec_f + O2 + alkoxy_fs

Forward k: 8.05E-16

This Reaction uses a Nonstandard Rate Law

Equation: hydrogen_abs => hydrogen_abs

Forward k: 1.0

This Reaction uses a Standard Rate Law

Equation: O_tert + H_sec => OH_tert + R_sec

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + H_sec_a => OH_tert + R_sec_a

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + H_sec_b => OH_tert + R_sec_b

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + H_beta => OH_tert + R_beta

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + H_beta_a => OH_tert + R_beta_a

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + H_tert => OH_tert + R_tert

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + H_tert_a => OH_tert + R_tert_a

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + OH_sec + H_sec_alc => R_OH_sec + OH_tert

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + OH_beta + H_beta_alc => R_OH_beta + OH_tert

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + OH_prim_f + H_prim_f => R_OH_prim_f + OH_tert

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + OC_prim_f + H_prim_f => R_OC_prim_f + OH_tert + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + OH_prim_f2 + H_prim_f2 => R_OH_prim_f2 + OH_tert

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + OC_prim_f2 + H_prim_f2 => R_OC_prim_f2 + OH_tert + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + OH_prim_f3 + H_prim_f3 => R_OH_prim_f3 + OH_tert

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + OC_prim_f3 + H_prim_f3 => R_OC_prim_f3 + OH_tert + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + 2 H_sec => OH_sec + R_sec + H_sec_alc

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_sec + H_sec_a => OH_sec + R_sec_a + H_sec_alc

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_sec + H_sec_b => OH_sec + R_sec_b + H_sec_alc

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_beta + H_sec => OH_sec + R_beta + H_sec_alc

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_beta_a + H_sec => OH_sec + R_beta_a + H_sec_alc

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_tert + H_sec => OH_sec + R_tert + H_sec_alc

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_tert_a + H_sec => OH_sec + R_tert_a + H_sec_alc

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + OH_sec + H_sec_alc + H_sec => R_OH_sec + OH_sec + H_sec_alc

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + OH_beta + H_beta_alc + H_sec => R_OH_beta + OH_sec + H_sec_alc

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + OH_prim_f + H_prim_f + H_sec => R_OH_prim_f + OH_sec + H_sec_alc

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + OC_prim_f + H_prim_f + H_sec => R_OC_prim_f + OH_sec + aldehyde_abs + H_sec_alc

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + OH_prim_f2 + H_prim_f2 + H_sec => R_OH_prim_f2 + OH_sec + H_sec_alc

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + OC_prim_f2 + H_prim_f2 + H_sec => R_OC_prim_f2 + OH_sec + aldehyde_abs + H_sec_alc

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + OH_prim_f3 + H_prim_f3 + H_sec => R_OH_prim_f3 + OH_sec + H_sec_alc

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + OC_prim_f3 + H_prim_f3 + H_sec => R_OC_prim_f3 + OH_sec + aldehyde_abs + H_sec_alc

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + H_sec + H_beta => OH_beta + R_sec + H_beta_alc

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + H_sec_a + H_beta => OH_beta + R_sec_a + H_beta_alc

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + H_sec_b + H_beta => OH_beta + R_sec_b + H_beta_alc

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + 2 H_beta => OH_beta + R_beta + H_beta_alc

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + H_beta + H_beta_a => OH_beta + R_beta_a + H_beta_alc

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + H_tert + H_beta => OH_beta + R_tert + H_beta_alc

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + H_tert_a + H_beta => OH_beta + R_tert_a + H_beta_alc

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + OH_sec + H_sec_alc + H_beta => R_OH_sec + OH_beta + H_beta_alc

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + OH_beta + H_beta_alc + H_beta => R_OH_beta + OH_beta + H_beta_alc

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + OH_prim_f + H_prim_f + H_beta => R_OH_prim_f + OH_beta + H_beta_alc

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + OC_prim_f + H_prim_f + H_beta => R_OC_prim_f + OH_beta + H_beta_alc + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + OH_prim_f2 + H_prim_f2 + H_beta => R_OH_prim_f2 + OH_beta + H_beta_alc

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + OC_prim_f2 + H_prim_f2 + H_beta => R_OC_prim_f2 + OH_beta + aldehyde_abs + H_beta_alc

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + OH_prim_f3 + H_prim_f3 + H_beta => R_OH_prim_f3 + OH_beta + H_beta_alc

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + OC_prim_f3 + H_prim_f3 + H_beta => R_OC_prim_f3 + OH_beta + aldehyde_abs + H_beta_alc

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f + H_sec => OH_prim_f + R_sec

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f + H_sec_a => OH_prim_f + R_sec_a

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f + H_sec_b => OH_prim_f + R_sec_b

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f + H_beta => OH_prim_f + R_beta

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f + H_beta_a => OH_prim_f + R_beta_a

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f + H_tert => OH_prim_f + R_tert

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f + H_tert_a => OH_prim_f + R_tert_a

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f + OH_sec + H_sec_alc => R_OH_sec + OH_prim_f

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f + OH_beta + H_beta_alc => R_OH_beta + OH_prim_f

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f + OH_prim_f + H_prim_f => R_OH_prim_f + OH_prim_f

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f + OC_prim_f + H_prim_f => R_OC_prim_f + OH_prim_f + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f + OH_prim_f2 + H_prim_f2 => R_OH_prim_f2 + OH_prim_f

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f + OC_prim_f2 + H_prim_f2 => R_OC_prim_f2 + OH_prim_f + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f + OH_prim_f3 + H_prim_f3 => R_OH_prim_f3 + OH_prim_f

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f + OC_prim_f3 + H_prim_f3 => R_OC_prim_f3 + OH_prim_f + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f2 + H_sec => OH_prim_f2 + R_sec

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f2 + H_sec_a => OH_prim_f2 + R_sec_a

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f2 + H_sec_b => OH_prim_f2 + R_sec_b

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f2 + H_beta => OH_prim_f2 + R_beta

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f2 + H_beta_a => OH_prim_f2 + R_beta_a

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f2 + H_tert => OH_prim_f2 + R_tert

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f2 + H_tert_a => OH_prim_f2 + R_tert_a

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f2 + OH_sec + H_sec_alc => R_OH_sec + OH_prim_f2

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f2 + OH_beta + H_beta_alc => R_OH_beta + OH_prim_f2

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f2 + OH_prim_f + H_prim_f => R_OH_prim_f + OH_prim_f2

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f2 + OC_prim_f + H_prim_f => R_OC_prim_f + OH_prim_f2 + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f2 + OH_prim_f2 + H_prim_f2 => R_OH_prim_f2 + OH_prim_f2

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f2 + OC_prim_f2 + H_prim_f2 => R_OC_prim_f2 + OH_prim_f2 + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f2 + OH_prim_f3 + H_prim_f3 => R_OH_prim_f3 + OH_prim_f2

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f2 + OC_prim_f3 + H_prim_f3 => R_OC_prim_f3 + OH_prim_f2 + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f3 + H_sec => OH_prim_f3 + R_sec

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f3 + H_sec_a => OH_prim_f3 + R_sec_a

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f3 + H_sec_b => OH_prim_f3 + R_sec_b

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f3 + H_beta => OH_prim_f3 + R_beta

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f3 + H_beta_a => OH_prim_f3 + R_beta_a

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f3 + H_tert => OH_prim_f3 + R_tert

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f3 + H_tert_a => OH_prim_f3 + R_tert_a

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f3 + OH_sec + H_sec_alc => R_OH_sec + OH_prim_f3

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f3 + OH_beta + H_beta_alc => R_OH_beta + OH_prim_f3

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f3 + OH_prim_f + H_prim_f => R_OH_prim_f + OH_prim_f3

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f3 + OC_prim_f + H_prim_f => R_OC_prim_f + OH_prim_f3 + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f3 + OH_prim_f2 + H_prim_f2 => R_OH_prim_f2 + OH_prim_f3

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f3 + OC_prim_f2 + H_prim_f2 => R_OC_prim_f2 + OH_prim_f3 + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f3 + OH_prim_f3 + H_prim_f3 => R_OH_prim_f3 + OH_prim_f3

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f3 + OC_prim_f3 + H_prim_f3 => R_OC_prim_f3 + OH_prim_f3 + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f4 + H_sec => OH_prim_f4 + R_sec

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f4 + H_sec_a => OH_prim_f4 + R_sec_a

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f4 + H_sec_b => OH_prim_f4 + R_sec_b

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f4 + H_beta => OH_prim_f4 + R_beta

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f4 + H_beta_a => OH_prim_f4 + R_beta_a

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f4 + H_tert => OH_prim_f4 + R_tert

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f4 + H_tert_a => OH_prim_f4 + R_tert_a

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f4 + OH_sec + H_sec_alc => R_OH_sec + OH_prim_f4

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f4 + OH_beta + H_beta_alc => R_OH_beta + OH_prim_f4

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f4 + OH_prim_f + H_prim_f => R_OH_prim_f + OH_prim_f4

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f4 + OC_prim_f + H_prim_f => R_OC_prim_f + OH_prim_f4 + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f4 + OH_prim_f2 + H_prim_f2 => R_OH_prim_f2 + OH_prim_f4

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f4 + OC_prim_f2 + H_prim_f2 => R_OC_prim_f2 + OH_prim_f4 + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f4 + OH_prim_f3 + H_prim_f3 => R_OH_prim_f3 + OH_prim_f4

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_prim_f4 + OC_prim_f3 + H_prim_f3 => R_OC_prim_f3 + OH_prim_f4 + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_f + H_sec => OH_sec_f + R_sec

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_f + H_sec_a => OH_sec_f + R_sec_a

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_f + H_sec_b => OH_sec_f + R_sec_b

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_f + H_beta => OH_sec_f + R_beta

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_f + H_beta_a => OH_sec_f + R_beta_a

Forward k: 3.77E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_f + H_tert => OH_sec_f + R_tert

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_f + H_tert_a => OH_sec_f + R_tert_a

Forward k: 7.55E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_f + OH_sec + H_sec_alc => R_OH_sec + OH_sec_f

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_f + OH_beta + H_beta_alc => R_OH_beta + OH_sec_f

Forward k: 1.29E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_f + OH_prim_f + H_prim_f => R_OH_prim_f + OH_sec_f

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_f + OC_prim_f + H_prim_f => R_OC_prim_f + OH_sec_f + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_f + OH_prim_f2 + H_prim_f2 => R_OH_prim_f2 + OH_sec_f

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_f + OC_prim_f2 + H_prim_f2 => R_OC_prim_f2 + OH_sec_f + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_f + OH_prim_f3 + H_prim_f3 => R_OH_prim_f3 + OH_sec_f

Forward k: 6.5E-17

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_f + OC_prim_f3 + H_prim_f3 => R_OC_prim_f3 + OH_sec_f + aldehyde_abs

Forward k: 2.45E-16

This Reaction uses a Nonstandard Rate Law

Equation: clock => clock

Forward k: 1.0

This Reaction uses a Standard Rate Law

Equation: Sq => SqO

Forward k: 1.28E-1

This Reaction uses a Standard Rate Law

Equation: SqO => SqO2

Forward k: 1.28E-1

This Reaction uses a Standard Rate Law

Equation: SqO2 => SqO3

Forward k: 1.28E-1

This Reaction uses a Standard Rate Law

Equation: SqO3 => SqO4

Forward k: 1.28E-1

This Reaction uses a Standard Rate Law

Equation: SqO4 => SqO5

Forward k: 1.28E-1

This Reaction uses a Standard Rate Law

Equation: carbon_act => carbon_act

Forward k: 1.0

This Reaction uses a Standard Rate Law

Equation: activate + C27 => a_C27

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: activate2 + C26 => a_C26

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: activate3 + C25 => a_C25

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: activate + C22 => a_C22

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: activate2 + C21 => a_C21

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: activate3 + C20 => a_C20

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: activate + C17 => a_C17

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: activate2 + C16 => a_C16

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: activate3 + C15 => a_C15

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: activate4 + C14 => a_C14

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: activate + C11 => a_C11

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: activate2 + C10 => a_C10

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: activate3 + C9 => a_C9

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: activate + C6 => a_C6

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: activate2 + C5 => a_C5

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: activate3 + C4 => a_C4

Forward k: 1E30

This Reaction uses a Nonstandard Rate Law

Equation: fragmentation => fragmentation

Forward k: 1.0

This Reaction uses a Standard Rate Law

Equation: O_tert + C30 + 2 H_sec_a => R_prim_f + 2 H_prim_f + C27 + OC_sec_f + C3 + alkoxy_f

Forward k: 2.21E4

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + C30 + 4 H_sec_a => R_prim_f + 2 H_prim_f + C6 + OC_sec_f + C24 + alkoxy_f + 2 H_sec

Forward k: 2.21E4

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + C30 + 4 H_sec_a => R_prim_f + 2 H_prim_f + C22 + OC_sec_f + C8 + alkoxy_f + 2 H_sec

Forward k: 2.21E4

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + C30 + 4 H_sec_a => R_prim_f + 2 H_prim_f + C11 + OC_sec_f + C19 + alkoxy_f + 2 H_sec

Forward k: 2.21E4

This Reaction uses a Nonstandard Rate Law

Equation: O_tert + C30 + 4 H_sec_a => R_prim_f + 2 H_prim_f + C17 + OC_sec_f + C13 + alkoxy_f + 2 H_sec

Forward k: 2.21E4

This Reaction uses a Nonstandard Rate Law

Equation: O_tert_a + C30 + OH_sec + H_sec_alc + 2 H_beta_a => R_OH_prim_f + H_prim_f + C27 + OC_sec_f + C3 + alkoxy_af + 2 H_beta

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_tert_a + C30 + OH_sec + H_sec_alc + 2 H_beta_a => R_OH_prim_f + H_prim_f + C22 + OC_sec_f + C8 + alkoxy_af + 2 H_beta

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_tert_a + C30 + OH_sec + H_sec_alc + 2 H_beta_a => R_OH_prim_f + H_prim_f + C17 + OC_sec_f + C13 + alkoxy_af + 2 H_beta

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_tert_a + C30 + OH_sec + H_sec_alc + 2 H_beta_a => R_OH_prim_f + H_prim_f + C11 + OC_sec_f + C19 + alkoxy_af + 2 H_beta

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_tert_a + C30 + OH_sec + H_sec_alc + 2 H_beta_a => R_OH_prim_f + H_prim_f + C6 + OC_sec_f + C24 + alkoxy_af + 2 H_beta

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_tert_a + C30 + OC_sec + 2 H_beta_a => R_OC_prim_f + C27 + OC_sec_f + C3 + alkoxy_af + 2 H_beta

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_tert_a + C30 + OC_sec + 2 H_beta_a => R_OC_prim_f + C22 + OC_sec_f + C8 + alkoxy_af + 2 H_beta

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_tert_a + C30 + OC_sec + 2 H_beta_a => R_OC_prim_f + C17 + OC_sec_f + C13 + alkoxy_af + 2 H_beta

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_tert_a + C30 + OC_sec + 2 H_beta_a => R_OC_prim_f + C11 + OC_sec_f + C19 + alkoxy_af + 2 H_beta

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_tert_a + C30 + OC_sec + 2 H_beta_a => R_OC_prim_f + C6 + OC_sec_f + C24 + alkoxy_af + 2 H_beta

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + C30 + H_beta + 4 H_sec_b => R_prim_f3 + 2 H_prim_f3 + C4 + OC_prim_f2 + H_prim_f2 + C26 + 2 H_sec + alkoxy_sf

Forward k: 2.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + C30 + H_beta + 4 H_sec_b => R_prim_f3 + 2 H_prim_f3 + C9 + OC_prim_f2 + H_prim_f2 + C21 + 2 H_sec + alkoxy_sf

Forward k: 2.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + C30 + H_beta + 4 H_sec_b => R_prim_f4 + 2 H_prim_f4 + C14 + OC_prim_f2 + H_prim_f2 + C16 + 2 H_beta + alkoxy_sf

Forward k: 2.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + C30 + H_beta + 4 H_sec_b => R_prim_f2 + 3 H_prim_f2 + 2 C15 + OC_prim_f2 + 2 H_sec + alkoxy_sf

Forward k: 2.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + C30 + H_beta + 4 H_sec_b => R_prim_f3 + 2 H_prim_f3 + C20 + OC_prim_f2 + H_prim_f2 + C10 + 2 H_sec + alkoxy_sf

Forward k: 2.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_beta + C30 + H_beta + 4 H_sec_b => R_prim_f3 + 2 H_prim_f3 + C25 + OC_prim_f2 + H_prim_f2 + C5 + 2 H_sec + alkoxy_sf

Forward k: 2.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_beta_a + C30 + OH_sec + H_sec_alc + H_tert_a + H_beta_a => R_OH_prim_f3 + H_prim_f3 + C4 + OC_prim_f2 + H_prim_f2 + C26 + H_tert + alkoxy_asf

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_beta_a + C30 + OH_sec + H_sec_alc + H_tert_a + H_beta_a => R_OH_prim_f3 + H_prim_f3 + C9 + OC_prim_f2 + H_prim_f2 + C21 + H_tert + alkoxy_asf

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_beta_a + C30 + OH_sec + H_sec_alc + H_tert_a + H_beta_a => R_OH_prim_f3 + H_prim_f3 + C20 + OC_prim_f2 + H_prim_f2 + C10 + H_tert + alkoxy_asf

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_beta_a + C30 + OH_sec + H_sec_alc + H_tert_a + H_beta_a => R_OH_prim_f3 + H_prim_f3 + C25 + OC_prim_f2 + H_prim_f2 + C5 + H_tert + alkoxy_asf

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_beta_a + C30 + OH_sec + H_sec_alc + H_tert_a + H_beta_a => R_OH_prim_f4 + H_prim_f4 + C14 + OC_prim_f2 + H_prim_f2 + C5 + H_tert + alkoxy_asf

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_beta_a + C30 + OC_sec + H_tert_a + H_beta_a => R_OC_prim_f3 + C4 + OC_prim_f2 + H_prim_f2 + C26 + H_tert + alkoxy_asf

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_beta_a + C30 + OC_sec + H_tert_a + H_beta_a => R_OC_prim_f3 + C9 + OC_prim_f2 + H_prim_f2 + C21 + H_tert + alkoxy_asf

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_beta_a + C30 + OC_sec + H_tert_a + H_beta_a => R_OC_prim_f3 + C20 + OC_prim_f2 + H_prim_f2 + C10 + H_tert + alkoxy_asf

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_beta_a + C30 + OC_sec + H_tert_a + H_beta_a => R_OC_prim_f3 + C25 + OC_prim_f2 + H_prim_f2 + C5 + H_tert + alkoxy_asf

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_beta_a + C30 + OC_sec + H_tert_a + H_beta_a => R_OC_prim_f4 + C14 + OC_prim_f2 + H_prim_f2 + C16 + H_tert + alkoxy_asf

Forward k: 3.6E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_tert_a + C30 + H_sec + 2 H_beta_a => R_sec_f + H_sec_f + C3 + OC_prim_f + H_prim_f + C27 + alkoxy_sf + 2 H_beta

Forward k: 3.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_tert_a + C30 + H_sec + 2 H_beta_a => R_sec_f + H_sec_f + C24 + OC_prim_f + H_prim_f + C6 + alkoxy_sf + 2 H_beta

Forward k: 3.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_tert_a + C30 + H_sec + 2 H_beta_a => R_sec_f + H_sec_f + C8 + OC_prim_f + H_prim_f + C22 + alkoxy_sf + 2 H_beta

Forward k: 3.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_tert_a + C30 + H_sec + 2 H_beta_a => R_sec_f + H_sec_f + C19 + OC_prim_f + H_prim_f + C11 + alkoxy_sf + 2 H_beta

Forward k: 3.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_tert_a + C30 + H_sec + 2 H_beta_a => R_sec_f + H_sec_f + C13 + OC_prim_f + H_prim_f + C17 + alkoxy_sf + 2 H_beta

Forward k: 3.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_tert_a + C30 + H_sec + 2 H_beta_a => R_prim_f2 + 2 H_prim_f2 + C5 + OC_prim_f3 + H_prim_f3 + C25 + alkoxy_sf + H_tert

Forward k: 1.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_tert_a + C30 + H_sec + 2 H_beta_a => R_prim_f2 + 2 H_prim_f2 + C10 + OC_prim_f3 + H_prim_f3 + C20 + alkoxy_sf + H_tert

Forward k: 1.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_tert_a + C30 + H_sec + 2 H_beta_a => R_prim_f2 + 2 H_prim_f2 + C16 + OC_prim_f4 + H_prim_f4 + C14 + alkoxy_sf + H_tert

Forward k: 1.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_tert_a + C30 + H_sec + 2 H_beta_a => R_prim_f2 + 2 H_prim_f2 + C21 + OC_prim_f3 + H_prim_f3 + C9 + alkoxy_sf + H_tert

Forward k: 1.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_sec + H_tert_a + C30 + H_sec + 2 H_beta_a => R_prim_f2 + 2 H_prim_f2 + C26 + OC_prim_f3 + H_prim_f3 + C4 + alkoxy_sf + H_tert

Forward k: 1.5E4

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_a + H_sec_a + C30 + OH_tert => R_OH_sec_f + C3 + OC_prim_f + H_prim_f + C27 + alkoxy_asf

Forward k: 2.7E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_a + 3 H_sec_a + C30 + OH_tert => R_OH_sec_f + C8 + OC_prim_f + H_prim_f + C22 + 2 H_sec + alkoxy_asf

Forward k: 2.7E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_a + 3 H_sec_a + C30 + OH_tert => R_OH_sec_f + C13 + OC_prim_f + H_prim_f + C17 + 2 H_sec + alkoxy_asf

Forward k: 2.7E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_a + 3 H_sec_a + C30 + OH_tert => R_OH_sec_f + C19 + OC_prim_f + H_prim_f + C11 + 2 H_sec + alkoxy_asf

Forward k: 2.7E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_a + 3 H_sec_a + C30 + OH_tert => R_OH_sec_f + C24 + OC_prim_f + H_prim_f + C6 + 2 H_sec + alkoxy_asf

Forward k: 2.7E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_b + 3 H_sec_b + H_beta_alc + C30 + OH_beta => R_OH_prim_f2 + H_prim_f2 + C26 + OC_prim_f3 + H_prim_f3 + C4 + 2 H_sec + alkoxy_asf

Forward k: 1.81E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_b + 3 H_sec_b + H_beta_alc + C30 + OH_beta => R_OH_prim_f2 + H_prim_f2 + C21 + OC_prim_f3 + H_prim_f3 + C9 + 2 H_sec + alkoxy_asf

Forward k: 1.81E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_b + 3 H_sec_b + H_beta_alc + C30 + OH_beta => R_OH_prim_f3 + 2 H_prim_f3 + 2 C15 + OC_prim_f3 + 2 H_sec + alkoxy_asf

Forward k: 1.81E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_b + 3 H_sec_b + H_beta_alc + C30 + OH_beta => R_OH_prim_f2 + H_prim_f2 + C16 + OC_prim_f4 + H_prim_f4 + C14 + 2 H_beta + alkoxy_asf

Forward k: 1.81E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_b + 3 H_sec_b + H_beta_alc + C30 + OH_beta => R_OH_prim_f2 + H_prim_f2 + C10 + OC_prim_f3 + H_prim_f3 + C20 + 2 H_sec + alkoxy_asf

Forward k: 1.81E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_b + 3 H_sec_b + H_beta_alc + C30 + OH_beta => R_OH_prim_f2 + H_prim_f2 + C5 + OC_prim_f3 + H_prim_f3 + C25 + 2 H_sec + alkoxy_asf

Forward k: 1.81E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_b + 3 H_sec_b + C30 + OC_beta => R_OC_prim_f2 + C26 + OC_prim_f3 + H_prim_f3 + C4 + 2 H_sec + alkoxy_asf

Forward k: 1.81E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_b + 3 H_sec_b + C30 + OC_beta => R_OC_prim_f2 + C21 + OC_prim_f3 + H_prim_f3 + C9 + 2 H_sec + alkoxy_asf

Forward k: 1.81E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_b + 3 H_sec_b + C30 + OC_beta => R_OC_prim_f3 + 2 C15 + OC_prim_f3 + H_prim_f3 + 2 H_sec + alkoxy_asf

Forward k: 1.81E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_b + 3 H_sec_b + C30 + OC_beta => R_OC_prim_f2 + C16 + OC_prim_f4 + H_prim_f4 + C14 + 2 H_beta + alkoxy_asf

Forward k: 1.81E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_b + 3 H_sec_b + C30 + OC_beta => R_OC_prim_f2 + C10 + OC_prim_f3 + H_prim_f3 + C20 + 2 H_sec + alkoxy_asf

Forward k: 1.81E9

This Reaction uses a Nonstandard Rate Law

Equation: O_sec_b + 3 H_sec_b + C30 + OC_beta => R_OC_prim_f2 + C5 + OC_prim_f3 + H_prim_f3 + C25 + 2 H_sec + alkoxy_asf

Forward k: 1.81E9

This Reaction uses a Nonstandard Rate Law

Equation: acyl_frag => acyl_frag

Forward k: 1.0

This Reaction uses a Standard Rate Law

Equation: O_OC_prim_f + a_C27 + 2 H_beta => CO2 + R_prim_f2 + C26 + 2 H_prim_f2

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: O_OC_prim_f2 + a_C26 + 2 H_sec => CO2 + R_prim_f3 + C25 + 2 H_prim_f3

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: O_OC_prim_f3 + a_C25 + H_tert => CO2 + R_sec_f + C24 + H_sec_f

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: O_OC_prim_f + a_C22 + 2 H_beta => CO2 + R_prim_f2 + C21 + 2 H_prim_f2

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: O_OC_prim_f2 + a_C21 + 2 H_sec => CO2 + R_prim_f3 + C20 + 2 H_prim_f3

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: O_OC_prim_f3 + a_C20 + H_tert => CO2 + R_sec_f + C19 + H_sec_f

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: O_OC_prim_f + a_C17 + 2 H_beta => CO2 + R_prim_f2 + C16 + 2 H_prim_f2

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: O_OC_prim_f2 + a_C16 + 2 H_beta => CO2 + R_prim_f3 + C15 + 2 H_prim_f3

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: O_OC_prim_f3 + a_C15 + 2 H_sec => CO2 + R_prim_f4 + C14 + 2 H_prim_f4

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: O_OC_prim_f4 + a_C14 + H_tert => CO2 + R_sec_f + C13 + H_sec_f

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: O_OC_prim_f + a_C11 + 2 H_beta => CO2 + R_prim_f2 + C10 + 2 H_prim_f2

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: O_OC_prim_f2 + a_C10 + 2 H_sec => CO2 + R_prim_f3 + C9 + 2 H_prim_f3

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: O_OC_prim_f3 + a_C9 + H_tert => CO2 + R_sec_f + C8 + H_sec_f

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: O_OC_prim_f + a_C6 + 2 H_beta => CO2 + R_prim_f2 + C5 + 2 H_prim_f2

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: O_OC_prim_f2 + a_C5 + 2 H_sec => CO2 + R_prim_f3 + C4 + 2 H_prim_f3

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: O_OC_prim_f3 + a_C4 + H_tert => CO2 + R_sec_f + C3 + H_sec_f

Forward k: 1E11

This Reaction uses a Nonstandard Rate Law

Equation: evaporation => evaporation

Forward k: 1.0

This Reaction uses a Standard Rate Law

Equation: OH_sec_f + C3 + 6 H_prim + H_sec_f => C3H8O_g

Forward k: 9.78E3

This Reaction uses a Nonstandard Rate Law

Equation: OC_sec_f + C3 + 6 H_prim => C3H6O_g

Forward k: 1.06E4

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f3 + C4 + 6 H_prim + H_tert + 2 H_prim_f3 => C4H10O_g

Forward k: 8.41E3

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f3 + C4 + 6 H_prim + H_tert + H_prim_f3 => C4H8O_g

Forward k: 1.03E4

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f2 + C5 + 6 H_prim + H_tert + 2 H_sec + 2 H_prim_f2 => C5H12O_g

Forward k: 5.94E3

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f2 + C5 + 6 H_prim + H_tert + 2 H_sec + H_prim_f2 => C5H10O_g

Forward k: 9.63E3

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f + C6 + 6 H_prim + H_tert + 2 H_sec + 2 H_beta + 2 H_prim_f => C6H14O_g

Forward k: 3.19E3

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f + C6 + 6 H_prim + H_tert + 2 H_sec + 2 H_beta + H_prim_f => C6H12O_g

Forward k: 5.33E3

This Reaction uses a Nonstandard Rate Law

Equation: OH_sec_f + C8 + 9 H_prim + H_sec_f + H_tert + 4 H_sec + 2 H_beta => C8H18O_g

Forward k: 5.12E2

This Reaction uses a Nonstandard Rate Law

Equation: OC_sec_f + C8 + 9 H_prim + 4 H_sec + 2 H_beta + H_tert => C8H16O_g

Forward k: 5.33E3

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f3 + C9 + 9 H_prim + 2 H_tert + 2 H_prim_f3 + 4 H_sec + 2 H_beta => C9H20O_g

Forward k: 1.83E2

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f3 + C9 + 9 H_prim + 2 H_tert + H_prim_f3 + 4 H_sec + 2 H_beta => C9H18O_g

Forward k: 1.26E3

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f2 + C10 + 9 H_prim + 2 H_tert + 2 H_prim_f2 + 6 H_sec + 2 H_beta => C10H22O_g

Forward k: 6.45E1

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f2 + C10 + 9 H_prim + 2 H_tert + H_prim_f2 + 6 H_sec + 2 H_beta => C10H20O_g

Forward k: 4.73E2

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f + C11 + 9 H_prim + 2 H_tert + 2 H_prim_f + 6 H_sec + 4 H_beta => C11H24O_g

Forward k: 2.26E1

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f + C11 + 9 H_prim + 2 H_tert + H_prim_f + 6 H_sec + 4 H_beta => C11H22O_g

Forward k: 1.7E2

This Reaction uses a Nonstandard Rate Law

Equation: OH_sec_f + C13 + 12 H_prim + 8 H_sec + 4 H_beta + 2 H_tert + H_sec_f => C13H28O_g

Forward k: 2.8

This Reaction uses a Nonstandard Rate Law

Equation: OC_sec_f + C13 + 12 H_prim + 8 H_sec + 4 H_beta + 2 H_tert => C13H26O_g

Forward k: 5.52E1

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f4 + C14 + 12 H_prim + 3 H_tert + 8 H_sec + 4 H_beta + 2 H_prim_f4 => C14H30O_g

Forward k: 9.87E-1

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f4 + C14 + 12 H_prim + 3 H_tert + 8 H_sec + 4 H_beta + H_prim_f4 => C14H28O_g

Forward k: 7.52

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f3 + C15 + 12 H_prim + 3 H_tert + 2 H_prim_f3 + 10 H_sec + 4 H_beta => C15H32O_g

Forward k: 3.49E-1

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f3 + C15 + 12 H_prim + 3 H_tert + H_prim_f3 + 10 H_sec + 4 H_beta => C15H30O_g

Forward k: 2.66

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f2 + C16 + 12 H_prim + 3 H_tert + 2 H_prim_f2 + 10 H_sec + 6 H_beta => C16H34O_g

Forward k: 1.23E-1

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f2 + C16 + 12 H_prim + 3 H_tert + H_prim_f2 + 10 H_sec + 6 H_beta => C16H32O_g

Forward k: 9.4E-1

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f + C17 + 12 H_prim + 3 H_tert + 2 H_prim_f + 10 H_sec + 8 H_beta => C17H36O_g

Forward k: 4.38E-2

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f + C17 + 12 H_prim + 3 H_tert + H_prim_f + 10 H_sec + 8 H_beta => C17H34O_g

Forward k: 3.33E-1

This Reaction uses a Nonstandard Rate Law

Equation: OH_sec_f + C19 + 15 H_prim + 12 H_sec + 8 H_beta + 3 H_tert + H_sec_f => C19H40O_g

Forward k: 5.53E-3

This Reaction uses a Nonstandard Rate Law

Equation: OC_sec_f + C19 + 15 H_prim + 12 H_sec + 8 H_beta + 3 H_tert => C19H38O_g

Forward k: 1.09E-1

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f3 + C20 + 15 H_prim + 4 H_tert + 2 H_prim_f3 + 12 H_sec + 8 H_beta => C20H42O_g

Forward k: 1.97E-3

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f3 + C20 + 15 H_prim + 4 H_tert + H_prim_f3 + 12 H_sec + 8 H_beta => C20H40O_g

Forward k: 1.50E-2

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f2 + C21 + 15 H_prim + 4 H_tert + 2 H_prim_f2 + 14 H_sec + 8 H_beta => C21H44O_g

Forward k: 7.02E-4

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f2 + C21 + 15 H_prim + 4 H_tert + H_prim_f2 + 14 H_sec + 8 H_beta => C21H42O_g

Forward k: 5.34E-3

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f + C22 + 15 H_prim + 4 H_tert + 2 H_prim_f + 14 H_sec + 10 H_beta => C22H46O_g

Forward k: 2.51E-4

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f + C22 + 15 H_prim + 4 H_tert + H_prim_f + 14 H_sec + 10 H_beta => C22H44O_g

Forward k: 1.91E-3

This Reaction uses a Nonstandard Rate Law

Equation: OH_sec_f + C24 + 18 H_prim + 16 H_sec + 10 H_beta + 4 H_tert + H_sec_f => C24H50O_g

Forward k: 3.2E-5

This Reaction uses a Nonstandard Rate Law

Equation: OC_sec_f + C24 + 18 H_prim + 16 H_sec + 10 H_beta + 4 H_tert => C24H48O_g

Forward k: 6.33E-4

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f3 + C25 + 18 H_prim + 5 H_tert + 2 H_prim_f3 + 16 H_sec + 10 H_beta => C25H52O_g

Forward k: 1.14E-5

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f3 + C25 + 18 H_prim + 5 H_tert + H_prim_f3 + 16 H_sec + 10 H_beta => C25H50O_g

Forward k: 8.7E-5

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f2 + C26 + 18 H_prim + 5 H_tert + 2 H_prim_f2 + 18 H_sec + 10 H_beta => C26H54O_g

Forward k: 4.10E-6

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f2 + C26 + 18 H_prim + 5 H_tert + H_prim_f2 + 18 H_sec + 10 H_beta => C26H52O_g

Forward k: 3.12E-5

This Reaction uses a Nonstandard Rate Law

Equation: OH_prim_f + C27 + 18 H_prim + 5 H_tert + 2 H_prim_f + 18 H_sec + 12 H_beta => C27H56O_g

Forward k: 1.47E-6

This Reaction uses a Nonstandard Rate Law

Equation: OC_prim_f + C27 + 18 H_prim + 5 H_tert + H_prim_f + 18 H_sec + 12 H_beta => C27H54O_g

Forward k: 1.12E-5

This Reaction uses a Nonstandard Rate Law