| | t0 | 0.00E+00 |
|----|---|----------|
| | tf | 9.00E-01 |
| 1 | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁] | 7.48E-01 |
| 2 | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH>[OQ'O ₁] | 7.48E-01 |
| 3 | $ [nR]O_{2}QOOH_{1} => OH+OQ'OOH_{1}>[OQ'OOH_{1}]OQ'OOH_{1} => OQ'O_{1}+OH\\ >[OQ'O_{1}]OQ'O_{1} => vinoxy+CH_{2}O>[vinoxy]vinoxy+O_{2} => CH_{2}O+CO+OH>[CO] $ | 7.48E-01 |
| 4 | >[OQ'O ₁]OQ'O ₁ =>vinoxy+CH ₂ O>[CH ₂ O]CH ₃ OO+CH ₂ O=>CH ₃ OOH+HCO >[CH ₃ OOH]CH ₃ OOH=>CH ₃ O+OH>[CH ₃ O] | 4.21E-02 |
| 5 | | 4.20E-02 |
| E | | 4.20E-02 |
| 7 | | 4.20E-02 |
| 8 | | 3.71E-02 |
| ğ | | 3.71E-02 |
| 10 | [nR]nROO+C ₃ H ₈ =>nROOH+iR>[nROOH]nROOH=>nRO+OH>[nRO] | 3.57E-02 |
| 11 | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH >[OQ'O ₁]OQ'O ₁ =>vinoxy+CH ₂ O>[CH ₂ O]iROO+CH ₂ O=>iROOH+HCO >[iROOH]iROOH=>iRO+OH>[iRO] | 3.14E-02 |
| 12 | | 3.13E-02 |

| | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH | |
|----------|--|----------|
| | >[OQ'O ₁]OQ'O ₁ =>vinoxy+CH ₂ O>[CH ₂ O]CH ₃ CH ₂ OO+CH ₂ O=>CH ₃ CH ₂ OOH+HCO | |
| 4.0 | >[CH ₃ CH ₂ OOH]CH ₃ CH ₂ OOH=>ethoxy+OH>[ethoxy]ethoxy=>CH ₃ +CH ₂ O | |
| 13 | >[CH ₃]CH ₃ OO+HO ₂ =>CH ₃ OOH+O ₂ >[CH ₃ OOH]CH ₃ OOH=>CH ₃ O+OH>[CH ₃ O] | 2.49E-02 |
| | | |
| | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH | |
| | $>[OQ'O_1]OQ'O_1=>vinoxy+CH_2O>[vinoxy]vinoxy+O_2=>CH_2O+CO+OH$ | |
| | >[CH ₂ O]CH ₃ CH ₂ OO+CH ₂ O=>CH ₃ CH ₂ OOH+HCO | |
| | >[CH ₃ CH ₂ OOH]CH ₃ CH ₂ OOH=>ethoxy+OH>[ethoxy]ethoxy=>CH ₃ +CH ₂ O | |
| 14 | >[CH ₃]CH ₃ OO+HO ₂ =>CH ₃ OOH+O ₂ >[CH ₃ OOH]CH ₃ OOH=>CH ₃ O+OH>[CH ₃ O] | 2.48E-02 |
| 15 | [nR]nROO+C ₃ H ₈ =>nROOH+nR>[nROOH]nROOH=>nRO+OH>[nRO] | 2.08E-02 |
| | | |
| | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH | |
| | $>[OQ'O_1]OQ'O_1=>vinoxy+CH_2O>[CH_2O]iROO+CH_2O=>iROOH+HCO$ | |
| | >[iROOH]iROOH=>iRO+OH>[iRO]iRO=>CH ₃ +acetaldehyde | |
| 16 | >[CH ₃]CH ₃ OO+HO ₂ =>CH ₃ OOH+O ₂ >[CH ₃ OOH]CH ₃ OOH=>CH ₃ O+OH>[CH ₃ O] | 1.90E-02 |
| | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH | |
| | >[OQ'O ₁]OQ'O ₁ =>vinoxy+CH ₂ O>[vinoxy]vinoxy+O ₂ =>CH ₂ O+CO+OH | |
| | >[CH ₂ O]iROO+CH ₂ O=>iROOH+HCO>[iROOH]iROOH=>iRO+OH | |
| | >[iRO]iRO=>CH ₃ +acetaldehyde>[CH ₃]CH ₃ OO+HO ₂ =>CH ₃ OOH+O ₂ | |
| 17 | >[CH ₃ OOH]CH ₃ OOH=>CH ₃ O+OH>[CH ₃ O] | 1.90E-02 |
| 18 | [nR]O ₂ QOOH ₁ =>HO ₂ +prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy] | 1.86E-02 |
| | [nR]nROO+C ₃ H ₈ =>nROOH+iR>[nROOH]nROOH=>nRO+OH | |
| | >[nRO]nRO=>C ₂ H ₅ +CH ₂ O>[C ₂ H ₅]CH ₃ CH ₂ OO+C ₃ H ₈ =>CH ₃ CH ₂ OOH+iR | |
| 19 | >[CH ₃ CH ₂ OOH]CH ₃ CH ₂ OOH=>ethoxy+OH>[ethoxy] | 9.54E-03 |
| 20 | [nR]nROO=>OH+propoxide>[propoxide] | 8.96E-03 |
| | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH | |
| | $>[OQ'O_1]OQ'O_1=>vinoxy+CH_2O>[vinoxy]vinoxy+O_2=>CH_2O+CO+OH$ | |
| | >[CH ₂ O]nROO+CH ₂ O=>nROOH+HCO>[nROOH]nROOH=>nRO+OH | |
| | >[nRO]nRO=>C ₂ H ₅ +CH ₂ O>[C ₂ H ₅]CH ₃ CH ₂ OO+HO ₂ =>CH ₃ CH ₂ OOH+O ₂ | |
| 21 | >[CH ₃ CH ₂ OOH]CH ₃ CH ₂ OOH=>ethoxy+OH>[ethoxy] | 8.60E-03 |
| | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH | |
| | >[OQ'O ₁]OQ'O ₁ =>vinoxy+CH ₂ O>[CH ₂ O]nROO+CH ₂ O=>nROOH+HCO | |
| | >[nROOH]nROOH=>nRO+OH>[nRO]nRO=>C ₂ H ₅ +CH ₂ O | |
| | $>[C_2H_5]CH_3CH_2OO+HO_2=>CH_3CH_2OOH+O_2>[CH_3CH_2OOH]CH_3CH_2OOH=>ethoxy+OH-O_2>[CH_3CH_2OOH]CH_3CH_2OOH=>ethoxy+OH-O_2>[CH_3CH_2OOH]CH_3CH_2OOH=>ethoxy+OH-O_2>[CH_3CH_2OOH]CH_3CH_2OOH=>ethoxy+OH-O_2>[CH_3CH_2OOH]CH_3CH_2OOH=>ethoxy+OH-O_2>[CH_3CH_2OOH]CH_3CH_2OOH=>ethoxy+OH-O_2>[CH_3CH_2OOH]CH_3CH_2OOH=>ethoxy+OH-O_2>[CH_3CH_2OOH]CH_3CH_2OOH=>ethoxy+OH-O_2>[CH_3CH_2OOH]CH_3CH_2OOH=>ethoxy+OH-O_2>[CH_3CH_2OOH]CH_3CH_2OOH=>ethoxy+OH-O_2>[CH_3CH_2OOH]CH_3CH_2OOH=>ethoxy+OH-O_2>[CH_3CH_2OOH]CH_2O$ | |
| 22 | ->[ethoxy] | 8.56E-03 |
| <u> </u> | | |

| | [nR]nROO=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide>[propoxide] | 6.29E-03 |
|----|--|----------|
| 24 | [nR]O ₂ +QOOH_1=>OH+OH+OQ'O ₁ >[OQ'O ₁] | 5.79E-0 |
| | [nR]O ₂ +QOOH_1=>OH+OH+OQ'O ₁ >[OQ'O ₁]OQ'O ₁ =>vinoxy+CH ₂ O | |
| 25 | >[vinoxy]vinoxy+O ₂ =>CH ₂ O+CO+OH>[CO] | 5.79E-0 |
| | [nR]nROO+C ₃ H ₈ =>nROOH+nR>[nROOH]nROOH=>nRO+OH | |
| | $>[nRO]nRO=>C_2H_5+CH_2O>[C_2H_5]CH_3CH_2OO+C_3H_8=>CH_3CH_2OOH+iR$ | |
| 26 | >[CH ₃ CH ₂ OOH]CH ₃ CH ₂ OOH=>ethoxy+OH>[ethoxy] | 5.57E-0 |
| | | |
| | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH | |
| | >[OQ'O ₁]OQ'O ₁ =>vinoxy+CH ₂ O>[CH ₂ O]nROO+CH ₂ O=>nROOH+HCO | |
| | >[nROOH]nROOH=>nRO+OH>[nRO]nRO=>C ₂ H ₅ +CH ₂ O | |
| | $>[C_2H_5]CH_3CH_2OO+HO_2=>CH_3CH_2OOH+O_2>[CH_3CH_2OOH]CH_3CH_2OOH=>ethoxy+OH-C_2H_3CH_2OOH=$ | |
| | ->[ethoxy]ethoxy=>CH ₃ +CH ₂ O>[CH ₃]CH ₃ OO+HO ₂ =>CH ₃ OOH+O ₂ | |
| 27 | >[CH ₃ OOH]CH ₃ OOH=>CH ₃ O+OH>[CH ₃ O] | 5.10E-03 |
| | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH | |
| | $>[OQ'O_1]OQ'O_1=>vinoxy+CH_2O>[CH_2O]iROO+CH_2O=>iROOH+HCO$ | |
| | >[iROOH]iROOH=>iRO+OH>[iRO]iRO=>CH ₃ +acetaldehyde | |
| | >[acetaldehyde]acetaldehyde+HO ₂ =>acetyl+H ₂ O ₂ | |
| | >[acetyl]acetyl(+M)=>CH ₃ +CO(+M)>[CH ₃]CH ₃ OO+HO ₂ =>CH ₃ OOH+O ₂ | |
| 28 | >[CH ₃ OOH]CH ₃ OOH=>CH ₃ O+OH>[CH ₃ O] | 3.76E-03 |
| | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH | |
| | >[OQ'O ₁]OQ'O ₁ =>vinoxy+CH ₂ O>[CH ₂ O]nROO+CH ₂ O=>nROOH+HCO | |
| | >[nROOH]nROOH=>nRO+OH>[nRO]nRO=>C ₂ H ₅ +CH ₂ O | |
| | >[C ₂ H ₅]CH ₃ CH ₂ OO+CH ₂ O=>CH ₃ CH ₂ OOH+HCO | |
| 29 | >[CH ₃ CH ₂ OOH]CH ₃ CH ₂ OOH=>ethoxy+OH>[ethoxy] | 3.69E-0 |
| | $ [nR] nROO => HO_2 + C_3H_6> [C_3H_6]C_3H_6 + OH => allyl + H_2O> [allyl]allyl + HO_2 => prod_2$ | |
| 30 | >[prod_2]prod_2=>allyloxy+OH>[allyloxy] | 3.45E-0 |
| | | |
| | | |
| | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH | |
| | >[OQ'O ₁]OQ'O ₁ =>vinoxy+CH ₂ O>[CH ₂ O]CH ₃ CH ₂ OO+CH ₂ O=>CH ₃ CH ₂ OOH+HCO | |
| | >[CH ₃ CH ₂ OOH]CH ₃ CH ₂ OOH=>ethoxy+OH>[ethoxy]ethoxy=>CH ₃ +CH ₂ O | |
| 31 | >[CH ₃]CH ₃ OO+CH ₂ O=>CH ₃ OOH+HCO>[CH ₃ OOH]CH ₃ OOH=>CH ₃ O+OH>[CH ₃ O] | 3.32E-0 |
| | [nR]nROO+C ₃ H ₈ =>nROOH+iR>[nROOH]nROOH=>nRO+OH | |
| | $>[nRO]nRO=>C_2H_5+CH_2O>[C_2H_5]CH_3CH_2OO+C_3H_8=>CH_3CH_2OOH+nR$ | |
| 32 | >[CH ₃ CH ₂ OOH]CH ₃ CH ₂ OOH=>ethoxy+OH>[ethoxy] | 3.19E-0 |
| 33 | [nR]nROO=>HO2+C3H6>[C3H6]C3H6+HO2=>propen1ol+OH>[propen1ol] | 3.00E-0 |

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| 34 | | 2.44E-03 |
| | $[nR]nROO+C_3H_8=>nROOH+iR>[nROOH]nROOH=>nRO+OH$ > $[nRO]nRO=>C_2H_5+CH_2O>[C_2H_5]CH_3CH_2OO+C_3H_8=>CH_3CH_2OOH+nR$ | |
| 35 | $>[nR]O_2QOOH_1=>OH+OQ'OOH_1>[OQ'OOH_1]OQ'OOH_1=>OQ'O_1+OH>[OQ'O_1]OQ'O_1=>vinoxy+CH_2O>[vinoxy]vinoxy+O_2=>CH_2O+CO+OH>[CO]$ | 2.44E-03 |
| | [nR]nROO+C ₃ H ₈ =>nROOH+iR>[nROOH]nROOH=>nRO+OH >[nRO]nRO=>C ₂ H ₅ +CH ₂ O>[C ₂ H ₅]CH ₃ CH ₂ OO+C ₃ H ₈ =>CH ₃ CH ₂ OOH+nR | |
| 36 | >[nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁] | 2.44E-03 |
| 37 | $ \label{eq:chcolor} $ | 2.06E-03 |
| 38 | $ [nR] nROO+C_3H_8=>nROOH+iR>[nROOH] nROOH=>nRO+OH \\ >[nRO] nRO=>C_2H_5+CH_2O>[CH_2O]CH_3CH_2OO+CH_2O=>CH_3CH_2OOH+HCO \\ >[CH_3CH_2OOH]CH_3CH_2OOH=>ethoxy+OH>[ethoxy] $ | 2.00E-03 |
| 39 | | 2.00E-03 |
| 40 | | 1.96E-03 |
| 41 | | 1.86E-03 |
| 42 | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH >[OQ'O ₁]OQ'O ₁ =>vinoxy+CH ₂ O>[vinoxy]vinoxy+O ₂ =>CH ₂ O+CO+OH >[CO]CO+HO ₂ =>CO ₂ +OH>[CO ₂] | 1.73E-03 |
| | $[nR]nROO => HO_2 + C_3H_6> [C_3H_6]HO_2 + C_3H_6 => OH + propoxide> [propoxide]$ | 1.57E-03 |
| | $[nR]nROO+C_3H_8=>nROOH+iR>[iR]iROO+C_3H_8=>iROOH+iR>[iROOH]iROOH=>iRO+OH>[iRO]$ | 1.50E-03 |
| 45 | [nR]O ₂ +QOOH_1=>HO ₂ +prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy] | 1.44E-03 |

| 46 | | 1.43E-03 |
|----|--|----------|
| 40 | | 1.431-03 |
| 47 | $ [nR]nROO+C_3H_8=>nROOH+nR>[nROOH]nROOH=>nRO+OH \\ >[nRO]nRO=>C_2H_5+CH_2O>[C_2H_5]CH_3CH_2OO+C_3H_8=>CH_3CH_2OOH+nR \\ >[nR]O_2QOOH_1=>OH+OQ'OOH_1>[OQ'OOH_1]OQ'OOH_1=>OQ'O_1+OH>[OQ'O_1] $ | 1.43E-03 |
| 48 | $ [nR]nROO+C_3H_8=>nROOH+nR>[nROOH]nROOH=>nRO+OH \\ >[nRO]nRO=>C_2H_5+CH_2O>[C_2H_5]CH_3CH_2OO+C_3H_8=>CH_3CH_2OOH+nR \\ >[nR]O_2QOOH_1=>OH+OQ'OOH_1>[OQ'OOH_1] $ | 1.43E-03 |
| 49 | $ [nR]O_2QOOH_1=>OH+OQ'OOH_1>[OQ'OOH_1]OQ'OOH_1=>OQ'O_1+OH\\ >[OQ'O_1]OQ'O_1=>vinoxy+CH_2O>[CH_2O]CH_2O+acetylperoxy=>HCO+CH_3CO_3H\\ >[CH_3CO_3H]CH_3CO_3H=>acetyloxy+OH>[acetyloxy]$ | 1.35E-03 |
| 50 | $ [nR]O_2QOOH_1=>OH+OQ'OOH_1>[OQ'OOH_1]OQ'OOH_1=>OQ'O_1+OH\\ >[OQ'O_1]OQ'O_1=>vinoxy+CH_2O>[vinoxy]vinoxy+O_2=>CH_2O+CO+OH\\ >[CH_2O]CH_2O+acetylperoxy=>HCO+CH_3CO_3H>[CH_3CO_3H]CH_3CO_3H=>acetyloxy+OH>[acetyloxy] $ | 1.35E-03 |
| 51 | | 1.23E-03 |
| 52 | | 1.21E-03 |
| | $ [nR]O_2QOOH_1=>OH+OQ'OOH_1>[OQ'OOH_1]OQ'OOH_1=>OQ'O_1+OH\\ >[OQ'O_1]OQ'O_1=>vinoxy+CH_2O>[vinoxy]vinoxy+O_2=>CH_2O+CO+OH\\ >[CH_2O]CH_2O+formylperoxy=>HCO+formylooh\\ >[formylooh]formylooh=>formyloxy+OH>[formyloxy] $ | 1.20E-03 |
| | $[nR]nROO=>HO_2+C_3H_6>[C_3H_6]C_3H_6+OH=>allyl+H_2O\\>[allyl]iROO+allyl=>iRO+allyloxy>[iRO]iRO=>CH_3+acetaldehyde\\>[CH_3]CH_3OO+HO_2=>CH_3OOH+O_2>[CH_3OOH]CH_3OOH=>CH_3O+OH>[CH_3O]$ | 1.20E-03 |
| 55 | $ [nR]nROO+C_3H_8=>nROOH+nR>[nROOH]nROOH=>nRO+OH \\ >[nRO]nRO=>C_2H_5+CH_2O>[CH_2O]CH_3CH_2OO+CH_2O=>CH_3CH_2OOH+HCO \\ >[CH_3CH_2OOH]CH_3CH_2OOH=>ethoxy+OH>[ethoxy] $ | 1.16E-03 |

| | [nR]nROO+C ₃ H ₈ =>nROOH+nR>[nROOH]nROOH=>nRO+OH | |
|----|--|----------|
| | >[nRO]nRO=>C ₂ H ₅ +CH ₂ O>[CH ₂ O]CH ₃ OO+CH ₂ O=>CH ₃ OOH+HCO | |
| 56 | >[CH ₃ OOH]CH ₃ OOH=>CH ₃ O+OH>[CH ₃ O] | 1.16E-03 |
| | [nR]nROO+C ₃ H ₈ =>nROOH+nR>[nROOH]nROOH=>nRO+OH | |
| | $>[nRO]nRO=>C_2H_5+CH_2O>[CH_2O]nROO+CH_2O=>nROOH+HCO$ | |
| 57 | >[nROOH]nROOH=>nRO+OH>[nRO] | 1.03E-03 |
| 58 | [nR]O ₂ +nR=>OH+propoxide>[propoxide] | 1.02E-03 |
| | [nR]O ₂ QOOH ₁ =>HO ₂ +prod_2>[prod_2]prod_2=>allyloxy+OH | |
| | >[allyloxy]allyloxy=>acrolein+H>[acrolein]acrolein+CH ₃ OO=>CH ₂ CHCO+CH ₃ OOH | |
| 59 | >[CH ₃ OOH]CH ₃ OOH=>CH ₃ O+OH>[CH ₃ O] | 1.01E-03 |
| | [nR]O ₂ QOOH ₁ =>OH+prod_3>[prod_3]prod_3=>frag_3+OH>[frag_3] | 9.71E-04 |
| | [nR]O ₂ QOOH ₁ =>OH+prod_3>[prod_3] | 9.71E-04 |
| | [nR]nROO+C ₃ H ₈ =>nROOH+nR>[nROOH]nROOH=>nRO+OH | |
| | >[nRO]nRO=>C ₂ H ₅ +CH ₂ O>[CH ₂ O]iROO+CH ₂ O=>iROOH+HCO | |
| 62 | >[iROOH]iROOH=>iRO+OH>[iRO] | 8.72E-04 |
| | | |
| | [nR]nROO+C ₃ H ₈ =>nROOH+iR>[nROOH]nROOH=>nRO+OH | |
| | >[nRO]nRO=>C ₂ H ₅ +CH ₂ O>[C ₂ H ₅]CH ₃ CH ₂ OO=>C ₂ H ₄ +HO ₂ | |
| 63 | >[C ₂ H ₄]C ₂ H ₄ +OH=>CH ₂ CH ₂ OH>[CH ₂ CH ₂ OH]O ₂ C ₂ H ₄ OH=>OH+CH ₂ O+CH ₂ O>[CH ₂ O] | 8.56E-04 |
| | | |
| | [nR]nROO+C ₃ H ₈ =>nROOH+iR>[nROOH]nROOH=>nRO+OH | |
| | $>[nRO]nRO=>C_2H_5+CH_2O>[C_2H_5]C_2H_5+O_2=>C_2H_4+HO_2$ | |
| 64 | >[C ₂ H ₄]C ₂ H ₄ +OH=>CH ₂ CH ₂ OH>[CH ₂ CH ₂ OH]O ₂ C ₂ H ₄ OH=>OH+CH ₂ O+CH ₂ O>[CH ₂ O] | 8.55E-04 |
| | [nR]O ₂ QOOH ₁ =>OH+prod_3>[prod_3]prod_3=>frag_3+OH | |
| 65 | >[frag_3]frag_3+OH=>prod_3>[prod_3]prod_3=>frag_3+OH>[frag_3] | 8.21E-04 |
| | $[nR]nROO=>HO_2+C_3H_6>[C_3H_6]C_3H_6+HO_2=>allyl+H_2O_2$ | |
| 66 | > <mark>[allyl]</mark> allyl+HO ₂ =>allyloxy+OH> <mark>[allyloxy]</mark> | 7.80E-04 |
| | | |
| | | |
| | [nR]O ₂ QOOH ₁ =>HO ₂ +prod_2>[prod_2]prod_2=>allyloxy+OH | |
| 67 | >[allyloxy]allyloxy=>acrolein+H>[acrolein]acrolein+CH ₃ OO=>CH ₂ CHCO+CH ₃ OOH | |
| 6/ | >[CH ₂ CHCO]CH ₂ CHCO+O ₂ =>vinoxy+CO ₂ >[vinoxy]vinoxy+O ₂ =>CH ₂ O+CO+OH>[CO] | 7.19E-04 |
| | $[nR]nROO = > HO_2 + C_3H_6 - > [C_3H_6]HO_2 + C_3H_6 = > QOOH_2 - QOOH_2 - QOOH_3 $ | 6 005 0 |
| 68 | >[QOOH_2]QOOH_2=>OH+propoxide>[propoxide] | 6.89E-04 |
| | | |
| 60 | [nR]nROO+ C_3H_8 =>nROOH+iR>[iR]iROO=> $HO_2+C_3H_6$ >[C_3H_6] C_3H_6+OH =>allyl+ H_2O- >[allyl]allyl+ HO_2 =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy] | 6.78E-04 |
| 09 | ~[aliyi]aliyi+1102-~pi0u_z~[pi0u_z]pi0u_z-~aliyi0xy+0N>[aliyi0xy] | U./OE-U4 |

| 70 | $ [nR]O_2QOOH_1=>OH+OQ'OOH_1>[OQ'OOH_1]OQ'OOH_1=>OQ'O_1+OH>[OQ'O_1]OQ'O_1=>vinoxy+CH_2O>[vinoxy]vinoxy+O_2=>CH_2O+CO+OH>[CH_2O]CH_2O+OH=>HCO+H_2O>[HCO]HCO+O_2=>formylperoxy>[formylperoxy]CH_2O+formylperoxy=>HCO+formylooh>[formylooh]formylooh=>formyloxy+OH>[formyloxy] $ | 5.91E-04 |
|----|---|----------|
| | $ [nR]O_2QOOH_1=>OH+OQ'OOH_1>[OQ'OOH_1]OQ'OOH_1=>OQ'O_1+OH>[OQ'O_1]OQ'O_1=>vinoxy+CH_2O>[CH_2O]CH_2O+OH=>HCO+H_2O>[HCO]HCO+O_2=>formylperoxy>[formylperoxy]CH_2O+formylperoxy=>HCO+formylooh$ | |
| 7: | >[formylooh]formylooh=>formyloxy+OH>[formyloxy] | 5.89E-04 |
| 72 | | 5.86E-04 |
| 73 | $ [nR]nROO => HO_2 + C_3H_6> [C_3H_6]H + C_3H_6 => nR> [nR]O_2QOOH_1 => OH + OQ'OOH_1 SOM + $ | 5.52E-04 |
| 74 | [nR]nROO=>HO ₂ +C ₃ H ₆ >[C ₃ H ₆]H+C ₃ H ₆ =>nR>[nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ ⁴ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH>[OQ'O ₁] | 5.48E-04 |
| 7! | | 5.48E-04 |
| 76 | [nR]O ₂ QOOH ₁ =>OH+prod_3>[prod_3]prod_3=>frag_3+OH >[frag_3]frag_3+OH=>prod_3>[prod_3]prod_3=>frag_3+OH >[frag_3]frag_3+OH=>prod_3>[prod_3]prod_3=>frag_3+OH>[frag_3] | 5.33E-04 |
| 77 | | 5.09E-04 |
| 78 | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH >[OQ'O ₁]OQ'O ₁ =>vinoxy+CH ₂ O>[CH ₂ O]CH ₂ O+OH=>HCO+H ₂ O 3>[HCO]HCO+O ₂ =>CO+HO ₂ >[CO]CO+HO ₂ =>CO ₂ +OH>[CO ₂] | 5.06E-04 |
| 79 | [nR]nROO+C ₃ H ₈ =>nROOH+nR>[nROOH]nROOH=>nRO+OH >[nRO]nRO=>C ₂ H ₅ +CH ₂ O>[C ₂ H ₅]CH ₃ CH ₂ OO=>C ₂ H ₄ +HO ₂ >[C ₂ H ₄]C ₂ H ₄ +OH=>CH ₂ CH ₂ OH>[CH ₂ CH ₂ OH]O ₂ C ₂ H ₄ OH=>OH+CH ₂ O+CH ₂ O>[CH ₂ O] | 5.00E-04 |
| 80 | | 4.95E-04 |

| | $[nR]O_2QOOH_1 = >OH + OQ'OOH_1> [OQ'OOH_1]OQ'OOH_1 = >OQ'O_1 + OH$ | |
|---|--|----------------------|
| | $>[OQ'O_1]OQ'O_1=>vinoxy+CH_2O>[vinoxy]vinoxy+O_2=>CH_2O+CO+OH$ | |
| | >[CH ₂ O]CH ₂ O+OH=>HCO+H ₂ O>[HCO]HCO+O ₂ =>formylperoxy | |
| | >[formylperoxy]C ₃ H ₈ +formylperoxy=>iR+formylooh | |
| 8 | 1 >[formylooh]formylooh=>formyloxy+OH>[formyloxy] | 4.86E-04 |
| | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH | |
| | | |
| | >[HCO]HCO+O ₂ =>formylperoxy | |
| | >[formylperoxy]C ₃ H ₈ +formylperoxy=>iR+formylooh | |
| Q | 2 >[formylooh]formylooh=>formyloxy+OH>[formyloxy] | 4.80E-04 |
| 0 | z >[totmyloon]totmyloon=>totmyloxy+OH>[totmyloxy] | 4.006-04 |
| | $[nR]nROO+C_3H_8=>nROOH+iR>[iR]iROO=>HO_2+C_3H_6>[C_3H_6]C_3H_6+HO_2=>allyl+H_2O_2-$ | |
| 0 | $\frac{1}{3} - \frac{1}{3} - \frac{1}$ | 3.78E-04 |
| 0 | $[nR] nROO = HO_2 + C_3H_6 - > [C_3H_6]H + C_3H_6 = > iR - > [iR] iROO + HO_2 = > iROOH + O_2 - > iROOH + O_3 - O_3$ | 3.76L-04 |
| o | | 2 455 04 |
| ŏ | 4 >[iROOH]iROOH=>iRO+OH>[iRO] | 3.45E-04 |
| | [nR]nROO+C ₃ H ₈ =>nROOH+iR> $[iR]$ iROO=>HO ₂ +C ₃ H ₆ | |
| 8 | 5 >[C ₃ H ₆]HO ₂ +C ₃ H ₆ =>OH+propoxide>[propoxide] | 3.09E-04 |
| | | |
| | [nR]O ₂ QOOH ₁ =>HO ₂ +prod_2>[prod_2]prod_2=>allyloxy+OH | |
| | >[allyloxy]allyloxy=>acrolein+H>[acrolein]acrolein+HO ₂ =>CH ₂ CHCO+H ₂ O ₂ | |
| | >[CH ₂ CHCO]CH ₂ CHCO= $>$ C ₂ H ₃ +CO $>$ [C ₂ H ₃]C ₂ H ₃ +O ₂ = $>$ O+vinoxy | |
| 8 | 6 >[vinoxy]vinoxy+O ₂ =>CH ₂ O+CO+OH>[CO] | 2.87E-04 |
| | | |
| | [nR]O ₂ QOOH ₁ =>HO ₂ +prod_2>[prod_2]prod_2=>allyloxy+OH | |
| | >[allyloxy]vinoxylmethyl=>acrolein+H>[acrolein]acrolein+HO ₂ =>CH ₂ CHCO+H ₂ O ₂ | |
| 8 | 7 >[CH ₂ CHCO]CH ₂ CHCO+O ₂ =>vinoxy+CO ₂ >[vinoxy]vinoxy+O ₂ =>CH ₂ O+CO+OH>[CO] | 2.72E-04 |
| | $[nR]O_2+nR=>HO_2+C_3H_6->[C_3H_6]C_3H_6+OH=>allyl+H_2O>[allyl]allyl+HO_2=>prod_2$ | |
| Q | 8 >[prod_2]prod_2=>allyloxy+OH>[allyloxy] | 2.70E-04 |
| | | 2.70L-04 |
| | [nR]O ₂ QOOH ₁ =>OH+prod_3>[prod_3]prod_3=>frag_3+OH | |
| | >[frag_3]frag_3+OH=>prod_3->[prod_3]prod_3=>frag_3+OH= | |
| o | >[frag_3]frag_3+OH=>prod_3>[prod_3]prod_3=>frag_3+OH 9 >[frag_3]frag_3+OH=>prod_3>[prod_3]prod_3=>frag_3+OH>[frag_3] | 2.65E-04 |
| | 0 [nR]O ₂ +nR=>HO ₂ +C ₃ H ₆ >[C ₃ H ₆]C ₃ H ₆ +HO ₂ =>propen1ol+OH>[propen1ol] | 2.03E-04 2.34E-04 |
| | | 2.34E-04 |
| 0 | [nR]nROO=>QOOH_2>[QOOH_2]well_2=>well_3 | 1.83E-04 |
| 9 | 1 >[well_3]QOOH_3=>OH+propoxide>[propoxide] | 1.03E-U4 |
| | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH | |
| _ | >[OQ'O ₁]OQ'O ₁ =>vinoxy+CH ₂ O>[CH ₂ O]CH ₂ O+HO ₂ =>HCO+H ₂ O ₂ | |
| 9 | 2 >[HCO]HCO+O ₂ =>CO+HO ₂ >[CO]CO+HO ₂ =>CO ₂ +OH>[CO ₂] | 1.53E-04 |
| | $[nR]O_2 + nR = > HO_2 + C_3H_6 - > [C_3H_6]C_3H_6 + HO_2 = > allyl + H_2O_2 - > [allyl]allyl + HO_2 = > prod_2 - > [allyl]allyl + HO_2 - > [$ | |
| 9 | 3 >[prod_2]prod_2=>allyloxy+OH>[allyloxy] | 1.50E-04 |

| 94 | [nR]O ₂ +nR=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide>[propoxide] | 1.45E-04 |
|----|---|----------|
| | [nR]O ₂ QOOH ₁ =>OH+OQ'OOH ₁ >[OQ'OOH ₁]OQ'OOH ₁ =>OQ'O ₁ +OH | |
| 95 | >[OQ'O ₁]OQ'O ₁ =>vinoxy+CH ₂ O>[CH ₂ O]CH ₂ O+O=>HCO+OH>[HCO] | 1.45E-04 |
| | [nR]nROO+C ₃ H ₈ =>nROOH+iR>[iR]iROO=>HO ₂ +C ₃ H ₆ >[C ₃ H ₆]HO ₂ +C ₃ H ₆ =>QOOH_2 | |
| 96 | >[QOOH_2]QOOH_2=>OH+propoxide>[propoxide] | 1.38E-04 |
| 97 | $[nR]O_2 + nR = > HO_2 + C_3H_6 - > [C_3H_6]HO_2 + C_3H_6 = > OH + propoxide - > [propoxide]$ | 1.22E-04 |
| | [nR]O ₂ QOOH ₁ =>OH+prod_3>[prod_3]prod_3=>frag_3+OH | |
| | >[frag_3]frag_3+OH=>prod_3>[prod_3]prod_3=>frag_3+OH | |
| | >[frag_3]frag_3+OH=>prod_3>[prod_3]prod_3=>frag_3+OH | |
| | >[frag_3]frag_3+OH=>prod_3>[prod_3]prod_3=>frag_3+OH | |
| 98 | >[frag_3]frag_3+OH=>prod_3>[prod_3]prod_3=>frag_3+OH>[frag_3] | 1.03E-04 |
| | $[nR]nROO = > HO_2 + C_3H_6 - > [C_3H_6]HO_2 + C_3H_6 = > QOOH_3 - $ | |
| 99 | >[QOOH_3]QOOH_3=>OH+propoxide>[propoxide] | 8.92E-05 |
| | [nR]QOOH_1=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide>[propoxide] | |