|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Reaction | Equation Format | SOHR Index |  |
| 1 | RH+O2=>nR+HO2 |  | 726 |  |
| 2 | RH+O2=>iR+HO2 |  | 724 |  |
| 3 | RH+OH=>nR+H2O |  | 736 |  |
| 4 | RH+OH=>iR+H2O |  | 738 |  |
| 5 | RH+HO2=>iR+H2O2 |  | 740 |  |
| 6 | iROO=>O2+iR |  | 1097 |  |
| 7 | O2QOOH1=>O2+QOOH1 |  | 1117 |  |
| 8 | RH+HO2=>nR+H2O2 |  | 742 |  |
| 9 | O2+iR=>HO2+C3H6 |  | 1100 |  |
| 10 | nROO=>O2+nR |  | 1069 |  |
| 11 | O2QOOH1=>OH+OQ′OOH1 |  | 1162 |  |
| 12 | nROO+RH=>nROOH+iR |  | 710 |  |
| 13 | iROO+RH=>iROOH+iR |  | 712 |  |
| 14 | iROO+RH=>iROOH+nR |  | 708 |  |
| 15 | HO2+HO2=>H2O2+O2 |  | 34 |  |
| 16 | iROO=>HO2+C3H6 |  | 1106 |  |
| 17 | iROOH=>iRO+OH |  | 716 |  |
| 18 | OQ′OOH1=>OQ′O1+OH |  | 1214 |  |
| 19 | CH3OO+RH=>CH3OOH+iR |  | 768 |  |
| 20 | nROOH=>nRO+OH |  | 714 |  |
| 21 | nROO+RH=>nROOH+nR |  | 706 |  |
| 22 | OQ′O1=>vinoxy+CH2O |  | 1222 |  |
| 23 | iRO=>CH3+acetaldehyde |  | 997 |  |
| 24 | CH3CH2OO+RH=>CH3CH2OOH+iR |  | 772 |  |
| 25 | nRO=>C2H5+CH2O |  | 993 |  |
| 26 | CH3OO+RH=>CH3OOH+nR |  | 766 |  |
| 27 | vinoxy+O2=>CH2O+CO+OH |  | 452 |  |
| 28 | O2+nR=>HO2+C3H6 |  | 1074 |  |
| 29 | CH3CH2OO+RH=>CH3CH2OOH+nR |  | 770 |  |
| 30 | CH3OO(+M)=>CH3+O2(+M) |  | 133 |  |
| 31 | CH3CH2OO=>C2H5+O2 |  | 349 |  |
| 32 | nROO=>HO2+C3H6 |  | 1082 |  |
| 33 | QOOH1=>O2+nR |  | 1073 |  |
| 34 | C2H5+O2=>C2H4+HO2 |  | 364 |  |
| 35 | iROO+HO2=>iROOH+O2 |  | 924 |  |
| 36 | O2+QOOH1=>OH+OH+OQ′O1 |  | 1118 |  |
| 37 | nROO+HO2=>nROOH+O2 |  | 922 |  |
| 38 | O2+iR=>OH+propoxide |  | 1102 |  |
| 39 | CH3OO+HO2=>CH3OOH+O2 |  | 142 |  |
| 40 | CH3OOH=>CH3O+OH |  | 154 |  |
| 41 | O2QOOH1=>HO2+prod2 |  | 1164 |  |
| 42 | CH3CH2OOH=>ethoxy+OH |  | 360 |  |
| 43 | H+RH=>H2+iR |  | 728 |  |
| 44 | QOOH3=>OH+propoxide |  | 1112 |  |
| 45 | O2+iR=>QOOH3 |  | 1098 |  |
| 46 | ethoxy=>CH3+CH2O |  | 345 |  |
| 47 | H+O2(+M)=>HO2(+M) |  | 24 |  |
| 48 | CH3O+M=>CH2O+H+M |  | 180 |  |
| 49 | iRO=>acetone+H |  | 615 |  |
| 50 | O2+nR=>OH+propoxide |  | 1076 |  |
| 51 | O2+QOOH1=>HO2+prod2 |  | 1120 |  |
| 52 | RH+CH3O=>nR+CH3OH |  | 762 |  |
| 53 | nROO=>OH+propoxide |  | 1084 |  |
| 54 | iROO+iROO=>O2+iRO+iRO |  | 966 |  |
| 55 | O2QOOH3=>O2 + QOOH3 |  | 1147 |  |
| 56 | O2 + QOOH3=>O2QOOH3 |  | 1146 |  |
| 57 | O2QOOH2=>O2 + QOOH2 |  | 1125 |  |
| 58 | O2 + QOOH2=>O2QOOH2 |  | 1124 |  |
| 59 | O2+QOOH1=>O2QOOH1 |  | 1116 |  |
| 60 | O2+iR=>iROO |  | 1096 |  |
| 61 | QOOH1=>nROO |  | 1081 |  |
| 62 | nROO=>QOOH1 |  | 1080 |  |
| 63 | O2+nR=>nROO |  | 1068 |  |
| 64 | vinoxylmethyl=>allyloxy |  | 1043 |  |
| 65 | allyloxy=>vinoxylmethyl |  | 1042 |  |
| 66 | CH2CH2OH+O2=>O2C2H4OH |  | 587 |  |
| 67 | O2C2H4OH=>CH2CH2OH+O2 |  | 586 |  |
| 68 | acetylperoxy=>acetyl+O2 |  | 435 |  |
| 69 | acetyl+O2=>acetylperoxy |  | 434 |  |
| 70 | C2H5+O2=>CH3CH2OO |  | 348 |  |
| 71 | CH3+O2(+M)=>CH3OO(+M) |  | 132 |  |
| 72 | CH3OO+CH2O=>CH3OOH+HCO |  | 134 |  |
| 73 | CH3CH2OO+CH2O=>CH3CH2OOH+HCO |  | 350 |  |
| 74 | iROO+CH2O=>iROOH+HCO |  | 918 |  |
| 75 | nROO+CH2O=>nROOH+HCO |  | 914 |  |
| 76 | HO2+C3H6=>OH+propoxide |  | 1114 |  |
| 77 | CH3CH2OO+HO2=>CH3CH2OOH+O2 |  | 356 |  |
| 78 | C3H6+HO2=>propen1ol+OH |  | 852 |  |
|  |  |  |  |  |

|  |  |  |  |
| --- | --- | --- | --- |
|  | 1 | 2 | 3 |
| Time 1 | Z5(iR, iROO) C3H6propen1ol | Z5(iR, iROO) iROOHiRO | Z5(iR, iROO) C3H6propoxide |
| Time 2 | Z5(iR, iROO) C3H6propen1ol | Z5(iR, iROO) iROOHiRO | Z5(iR, iROO) C3H6propoxide |
| Time 3 | Z5(iR, iROO) C3H6propen1ol | Z5(iR, iROO) iROOHiRO | Z5(iR, iROO) C3H6propoxide |
| Time 4 | Z5(iR, iROO) iROOHiRO | Z5(iR, iROO) C3H6propen1ol | Z5(iR, iROO) iROOHiRO |
| Time 5 | Z5(iR, iROO) iROOHiRO | Z5(iR, iROO) C3H6propen1ol | Z5(iR, iROO) iROOHiRO |
| Time 6 | Z5(iR, iROO) iROOHiRO | Z5(iR, iROO) C3H6propen1ol | Z5(iR, iROO) iROOHiRO |
| Time 7 | Z5(iR, iROO) iROOHiRO | Z5(iR, iROO) C3H6propen1ol | Z5(iR, iROO) iROOHiRO Z1(CH3, CH3OO) CH3OOHCH3O |
| Time 8 | Z5(iR, iROO) iROOHiRO | Z5(iR, iROO) iROOHiRO Z1(CH3, CH3OO) CH3OOHCH3O | Z5(iR, iROO) C3H6propen1ol |
| Time 9 | Z5(iR, iROO) iROOHiRO | Z5(iR, iROO) iROOHiRO | Z5(iR, iROO) C3H6propen1ol |

HO2 (middle time)> CH2O (late time)> RH (early time)

Z4(nR, O2QOOH1)

Z5(iR, iROO)

Z1(CH3, CH3OO)

Z2(C2H5, CH3CH2OO)

propen1ol, (check from the link below)

https://pubchem.ncbi.nlm.nih.gov/compound/5463330#section=Top

