|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Species Index | Old Species Name | New Species Name | Old Reaction Index | New Reaction Index | Primary Reaction |
| Group 1 |  |  |  |  |  |
| 25 | CH3 |  | 69 | 132 | CH3+O2(+M)=>CH3OO(+M) |
| 27 | CH3OO |  | -69 | 133 | CH3OO(+M)=>CH3+O2(+M) |
| Group 2 |  |  |  |  |  |
| 39 | C2H5 |  | 180 | 348 | C2H5+O2=>CH3CH2OO |
| 50 | CH3CH2OO |  | -180 | 349 | CH3CH2OO=>C2H5+O2 |
| Group 3 |  |  |  |  |  |
| 45 | Acetyl |  | 224 | 434 | acetyl+O2=>acetylperoxy |
| 47 | Acetylperoxy |  | -224 | 435 | acetylperoxy=>acetyl+O2 |
| Group 4 |  |  |  |  |  |
| 60 | npropyl | nR | 549 | 1068 | O2+npropyl=>npropyloo |
| 78 | npropyloo | nROO | -549 | 1069 | npropyloo=>O2+npropyl |
|  |  |  | 556,557 | 1080 | npropyloo=>QOOH\_1 |
|  |  |  | -556,-557 | 1081 | QOOH\_1=>npropyloo |
| 87 | QOOH\_1 |  | 575 | 1116 | O2+QOOH\_1=>well\_1 |
| 90 | well\_1 | O2QOOH1 | -575 | 1117 | well\_1=>O2+QOOH\_1 |
| Group 5 |  |  |  |  |  |
| 61 | ipropyl | iR | 565 | 1096 | O2+ipropyl=>ipropyloo |
| 80 | ipropyloo | iROO | -565 | 1097 | ipropyloo=>O2+ipropyl |
| Group 6 |  |  |  |  |  |
| 72 | allyloxy |  | 536 | 1042 | allyloxy=>vinoxylmethyl |
| 108 | vinoxylmethyl |  | -536 | 1043 | vinoxylmethyl=>allyloxy |
| Group 7 |  |  |  |  |  |
| 85 | O2C2H4OH |  | 300 | 586 | O2C2H4OH=>CH2CH2OH+O2 |
| 54 | CH2CH2OH |  | -300 | 587 | CH2CH2OH+O2=>O2C2H4OH |
| Group 8 |  |  |  |  |  |
| 88 | QOOH\_2 |  | 579 | 1124 | O2 + QOOH\_2=>well\_2 |
| 91 | well\_2 | O2QOOH2 | -579 | 1125 | well\_2=>O2 + QOOH\_2 |
| Group 9 |  |  |  |  |  |
| 89 | QOOH\_3 |  | 590 | 1146 | O2 + QOOH\_3=>well\_3 |
| 92 | well\_3 | O2QOOH3 | -590 | 1147 | well\_3=>O2 + QOOH\_3 |