| Proposed New San Diego Mechanism | | | | |
|---|---|---|---|---|
| **REACTIONS** | **A** | **n** | **E (cal/mol)** | **Note** |
| O+N2<=>NO+N | 1.47E+13 | 0.3 | 75286.81 | No Change |
| N+O2<=>NO+O | 6.40E+09 | 1 | 6285.85 | No Change |
| N+OH<=>NO+H | 3.80E+13 | 0 | 0 | No Change |
| NH+H<=>N+H2 | 1.00E+14 | 0 | 0 | J.A. Miller et al. PECS, 15 (1989) 287<br>More Recent Data, was Too Low |
| NH+O<=>NO+H | 9.20E+13 | 0 | 0 | No Change |
| NH+OH<=>HNO+H | 4.00E+13 | 0 | 0 | No Change |
| NH+OH<=>N+H2O | 5.00E+11 | 0.5 | 2000.48 | No Change |
| NH+O2<=>HNO+O | 4.60E+05 | 2 | 6500.96 | No Change |
| NH+NO<=>N2O+H | 1.80E+14 | -0.351 | -244 | P. Glarborg et al., CNF, 115 (1998) 1<br>More Recent Data, was Too Low |
| NH+NO<=>N2+OH | 2.20E+13 | -0.23 | 0 | No Change |
| NH2+H<=>NH+H2 | 4.00E+13 | 0 | 3652.01 | No Change |
| NH2+O<=>HNO+H | 6.60E+14 | -0.5 | 0 | P. Glarborg et al., CNF, 115 (1998) 1<br>More Recent Data, was Too High |
| NH2+OH<=>NH+H2O | 4.00E+06 | 2 | 1001.43 | No Change |
| NH2+NO<=>N2+H2O | 2.80E+20 | 2.654 | 1258 | J.A. Miller et al., IJCK, 1999, 31, 757.<br>More Recent Data, was Too Low |
| NH2+NO<=>N2H+OH | 3.10E+13 | -0.48 | 1180 | P. Glarborg et al., CNF, 115 (1998) 1<br>More Recent Data, was Too High |
| NH3+M<=>NH2+H+M<br>Unity Efficiencies | 2.20E+16 | 0 | 93451.24 | No Change |
| NH3+H<=>NH2+H2 | 6.40E+05 | 2.39 | 10181.64 | No Change |
| NH3+O<=>NH2+OH | 9.40E+06 | 1.94 | 6465.11 | No Change |
| NH3+OH<=>NH2+H2O | 2.04E+06 | 2.04 | 566.44 | No Change |
| N2H(+M)=N2+H(+M) (Lindemann Falloff) HPL | 6.50E+07 | 0 | 0 | J.A. Miller et al., IJCK, 1999, 31, 757. |
| Unity Efficiencies LPL | 5.00E+13 | 0 | 0 | Previously LPL Only and Too High |
| N2H+O<=>N2O+H | 1.00E+14 | 0 | 0 | No Change |
| N2H+OH<=>N2+H2O | 5.00E+13 | 0 | 0 | No Change |
| H+NO+M<=>HNO+M (Lindemann Falloff) HPL | 1.50E+15 | -0.4 | 0.00E+00 | P.Dagaut et al. PECS, 34 (2008) 1-46 |
| N2/2.00/ O2/2.00/ H2/2.00/ H2O/10.00/ LPL | 2.30E+14 | 0.206 | -1554.97 | Previously Reverse, LPL Only, and Too Low |
| HNO+H<=>NO+H2 | 4.40E+11 | 0.72 | 650.1 | No Change |
| HNO+OH<=>NO+H2O | 3.60E+13 | 0 | 0 | No Change |
| N2O(+M)<=>N2+O(+M) (Lindemann Falloff) HPL | 8.00E+11 | 0 | 62619.5 | No Change |
| Unity Efficiencies LPL | 2E+14 | 0 | 56644.36 | |
| N2O+H<=>N2+OH | 3.31E+10 | 0 | 5.09E+03 | D. L. Baulch et al., JPC, 34 (2005) 757-1397 |
| DUP | 7.83E+14 | 0 | 19390 | Previously Not Duplicated and Too Low |
| N2O+O<=>2 NO | 9.15E+13 | 0 | 27693 | Meagher et al. JPC, A 2000, 104, 6013<br>More Recent Data, was Too High |
| N2O+OH<=>N2+HO2 | 2.00E+12 | 0 | 40000 | Mueller et al. IJCK, 32 (2000) 317<br>More Recent Data, was Too High |
| NO2+M<=>NO+O+M<br>H2O/16.25/ | 1.10E+16 | 0 | 65965.58 | No Change |
| NO+HO2<=>NO2+OH | 2.10E+12 | 0 | -480.4 | No Change |
| NO2+H<=>NO+OH | 3.50E+14 | 0 | 1500.96 | No Change |
| NO2+O<=>NO+O2 | 1.00E+13 | 0 | 599.9 | No Change |
| **2 New Steps (Sensitivity Coeffcients > 10^-2) Added to Improve Flame Speed Calculation** | | | | |
| NH2+N<=>N2+H+H | 7.00E+13 | 0 | 0 | Glarborg P et al., CNF, 1998;115:1 |
| N2H+O2<=>N2+HO2 | 2.00E+14 | 0 | 0 | Glarborg P et al., CNF, 1998;115:1 |
| **4 New Steps Added to Improve the Ignition Delay Time Calculation** | | | | |
| NH2+O2<=>HNO+OH | 6.20E+07 | 1.20E+00 | 35099.9044 | Dean A et al. GCC, 2000; p. 125–341. |
| NH2+O2<=>H2NO+O | 2.50E+11 | 4.80E-01 | 29586 | Dean A et al. GCC, 2000; p. 125–341. |
| H2NO+O<=>HNO+OH | 3.00E+07 | 2.00E+00 | 2000 | Glarborg P et al., CNF, 1998;115:1 |
| H2NO+O2<=>HNO+HO2 | 3.00E+12 | 0.00E+00 | 25000 | J.A. Miller et al., IJCK, 1999, 31, 757. |