**Part 1: Naphthalene chemical scheme**

**Part 2: Modeling data**

# Part 1: Naphthalene chemical scheme

## Table S1: Stable species list and properties

| Name | MW (g mol$^{-1}$) | nbC | nbH | nbO | nbN | Chem code (GECKO-A) | Smile code | $P^{sat}$ (torr) | $\Delta H^{vap}$ (kJ) |
|---|---|---|---|---|---|---|---|---|---|
| **CH2O** | 30. | 1 | 2 | 1 | 0 | CH2O | C(=O) | - | - |
| **CHOOH** | 46. | 1 | 2 | 2 | 0 | CHO(OH) | C(=O)(O) | - | - |
| **DH** | 76. | 2 | 4 | 3 | 0 | CHOCH2(OOH) | O=CC(OO) | 0.112E+01 | 55.3 |
| **DO** | 60. | 2 | 4 | 2 | 0 | CHOCH2(OH) | O=CC(O) | 0.769E+01 | 47.7 |
| **GLYA** | 74. | 2 | 2 | 3 | 0 | CHOCO(OH) | O=CC(=O)(O) | 0.589E+00 | 58.6 |
| **GLYG** | 90. | 2 | 2 | 4 | 0 | CHOCO(OOH) | O=CC(=O)(OO) | 0.207E+01 | 53.2 |
| **GLYOX** | 58. | 2 | 2 | 2 | 0 | CHOCHO | O=CC=O | 0.289E+01 | 50.7 |
| **HPh** | 110. | 6 | 6 | 2 | 0 | c1HcHcHcHcHc1(OOH) | c1ccccc1(OO) | 0.530E-01 | 66.0 |
| **HPhA** | 154. | 7 | 6 | 4 | 0 | CO(OH)c1cHcHcHcHc1(OOH) | C(=O)(O)c1ccccc1(OO) | 0.993E-06 | 115.6 |
| **HPhD** | 138. | 7 | 6 | 3 | 0 | CHOc1cHcHcHcHc1(OOH) | C(=O)c1ccccc1(OO) | 0.952E-03 | 82.9 |
| **HPhKA** | 182. | 8 | 6 | 5 | 0 | c1(OOH)cHcHcHcHc1COCO(OH) | c1(OO)ccccc1C(=O)C(=O)(O) | 0.313E-07 | 130.9 |
| **HPhKKA** | 210. | 9 | 6 | 6 | 0 | c1(OOH)cHcHcHcHc1COCOCO(OH) | c1(OO)ccccc1C(=O)C(=O)C(=O)(O) | 0.383E-09 | 151.5 |
| **HPhKOA** | 212. | 9 | 8 | 6 | 0 | c1(OOH)cHcHcHcHc1COCH(OH)CO(OH) | c1(OO)ccccc1C(=O)C(O)C(=O)(O) | 0.184E-10 | 167.3 |
| **HPhOA** | 184. | 8 | 8 | 5 | 0 | c1(OOH)cHcHcHcHc1CH(OH)CO(OH) | c1(OO)ccccc1C(O)C(=O)(O) | 0.101E-08 | 148.8 |
| **HPhOUA** | 196. | 9 | 8 | 5 | 0 | c1(OOH)cHcHcHcHc1Cd(OH)=CdHCO(OH) | c1(OO)ccccc1C(O)=CC(=O)(O) | 0.791E-10 | 160.7 |
| **HPhUA** | 180. | 9 | 8 | 4 | 0 | c1(OOH)cHcHcHcHc1CdH=CdHCO(OH) | c1(OO)ccccc1C=CC(=O)(O) | 0.131E-07 | 135.2 |
| **NaH** | 160. | 10 | 8 | 2 | 0 | c12cHcHcHcHc1cHcHcHc2(OOH) | c12ccccc1cccc2(OO) | 0.842E-07 | 122.8 |
| **NaHKON** | 255. | 10 | 9 | 7 | 1 | c12cHcHcHcHc1CH(ONO2)CH(OOH)CH(OH)C2O | c12ccccc1C(ON(=O)=O)C(OO)C(O)C2=O | 0.641E-09 | 149.5 |
| **NaHO** | 176. | 10 | 8 | 3 | 0 | c12cHcHcHcHc1cHcHc(OOH)c2(OH) | c12ccccc1ccc(OO)c2(O) | 0.365E-09 | 149.1 |
| **NaHOOK** | 210. | 10 | 10 | 5 | 0 | c12cHcHcHcHc1COCH(OH)CH(OOH)C2H(OH) | c12ccccc1C(=O)C(O)C(OO)C2(O) | 0.742E-09 | 149.5 |
| **NaKK** | 158. | 10 | 6 | 2 | 0 | c12cHcHcHcHc1CdH=CdHCOC2O | c12ccccc1C=CC(=O)C2=O | 0.394E-02 | 72.9 |
| **NaKKON** | 237. | 10 | 7 | 6 | 1 | c12cHcHcHcHc1CH(ONO2)COCH(OH)C2O | c12ccccc1C(ON(=O)=O)C(=O)C(O)C2=O | 0.146E-06 | 122.8 |
| **NaNKON** | 284. | 10 | 8 | 8 | 2 | c12cHcHcHcHc1CH(ONO2)CH(ONO2)CH(OH)C2O | c12ccccc1C(ON(=O)=O)C(ON(=O)=O)C(O)C2=O | 0.107E-07 | 135.7 |
| **NaNOOK** | 239. | 10 | 9 | 6 | 1 | c12cHcHcHcHc1COCH(OH)CH(ONO2)C2H(OH) | c12ccccc1C(=O)C(O)C(ON(=O)=O)C2(O) | 0.129E-07 | 135.7 |
| **NaO** | 144. | 10 | 8 | 1 | 0 | c12cHcHcHcHc1cHcHcHc2(OH) | c12ccccc1cccc2(O) | 0.600E-05 | 102.0 |
| **NaOHBp** | 242. | 10 | 10 | 7 | 0 | c12cHcHcHcHc1CH(OOH)C3HCH(OH)C2H-O--O3- | c12ccccc1C(OO)C3C(O)C2OO3 | 0.231E-04 | 102.2 |

| Name | MW (g mol$^{-1}$) | nbC | nbH | nbO | nbN | Chem code (GECKO-A) | Smile code | $P^{sat}$ (torr) | $\Delta H^{vap}$ (kJ) |
|---|---|---|---|---|---|---|---|---|---|
| **NaOHort** | 178. | 10 | 10 | 3 | 0 | c12cHcHcHcHc1CdH=CdHCH(OOH)C2H(OH) | c12ccccc1C=CC(OO)C2(O) | 0.221E-05 | 111.0 |
| **NaOHpar** | 178. | 10 | 10 | 3 | 0 | c12cHcHcHcHc1CH(OOH)CdH=CdHC2H(OH) | c12ccccc1C(OO)C=CC2(O) | 0.221E-05 | 111.0 |
| **NaOKBp** | 224. | 10 | 8 | 6 | 0 | c12cHcHcHcHc1COC3HCH(OH)C2H-O--O3- | c12ccccc1C(=O)C3C(O)C2OO3 | 0.296E-02 | 78.2 |
| **NaOKKH** | 208. | 10 | 8 | 5 | 0 | c12cHcHcHcHc1CH(OH)CH(OOH)COC2O | c12ccccc1C(O)C(OO)C(=O)C2=O | 0.974E-08 | 135.9 |
| **NaOKKK** | 190. | 10 | 6 | 4 | 0 | c12cHcHcHcHc1CH(OH)COCOC2O | c12ccccc1C(O)C(=O)C(=O)C2=O | 0.188E-05 | 110.1 |
| **NaOKKN** | 237. | 10 | 7 | 6 | 1 | c12cHcHcHcHc1CH(OH)CH(ONO2)COC2O | c12ccccc1C(O)C(ON(=O)=O)C(=O)C2=O | 0.146E-06 | 122.8 |
| **NaOKON** | 239. | 10 | 9 | 6 | 1 | c12cHcHcHcHc1CH(ONO2)CH(OH)CH(OH)C2O | c12ccccc1C(ON(=O)=O)C(O)C(O)C2=O | 0.129E-07 | 135.7 |
| **NaOKort** | 160. | 10 | 8 | 2 | 0 | c12cHcHcHcHc1CdH=CdHCH(OH)C2O | c12ccccc1C=CC(O)C2=O | 0.607E-03 | 83.4 |
| **NaOKpar** | 160. | 10 | 8 | 2 | 0 | c12cHcHcHcHc1COCdH=CdHC2H(OH) | c12ccccc1C(=O)C=CC2(O) | 0.448E-03 | 84.5 |
| **NaONBp** | 271. | 10 | 9 | 8 | 1 | c12cHcHcHcHc1CH(ONO2)C3HCH(OH)C2H-O--O3- | c12ccccc1C(ON(=O)=O)C3C(O)C2OO3 | 0.122E-03 | 94.3 |
| **NaONort** | 207. | 10 | 9 | 4 | 1 | c12cHcHcHcHc1CdH=CdHCH(ONO2)C2H(OH) | c12ccccc1C=CC(ON(=O)=O)C2(O) | 0.229E-04 | 100.3 |
| **NaONpar** | 207. | 10 | 9 | 4 | 1 | c12cHcHcHcHc1CH(ONO2)CdH=CdHC2H(OH) | c12ccccc1C(ON(=O)=O)C=CC2(O) | 0.229E-04 | 100.3 |
| **NaOO** | 160. | 10 | 8 | 2 | 0 | c12cHcHcHcHc1cHcHc(OH)c2(OH) | c12ccccc1ccc(O)c2(O) | 0.398E-07 | 125.8 |
| **NaOOBp** | 226. | 10 | 10 | 6 | 0 | c12cHcHcHcHc1CH(OH)C3HCH(OH)C2H-O--O3- | c12ccccc1C(O)C3C(O)C2OO3 | 0.317E-03 | 90.9 |
| **NaOOHBp** | 258. | 10 | 10 | 8 | 0 | c12cHcHcHcHc1CH(OOH)C3HCH(OH)C2(OH)-O--O3- | c12ccccc1C(OO)C3C(O)C2(O)OO3 | 0.313E-06 | 123.5 |
| **NaOOHort** | 194. | 10 | 10 | 4 | 0 | c12cHcHcHcHc1CH(OH)CH(OOH)CdH=Cd2(OH) | c12ccccc1C(O)C(OO)C=C2(O) | 0.217E-07 | 134.2 |
| **NaOOK** | 176. | 10 | 8 | 3 | 0 | c12cHcHcHcHc1Cd(OH)=CdHCH(OH)C2O | c12ccccc1C(O)=CC(O)C2=O | 0.705E-05 | 106.0 |
| **NaOOKBp** | 240. | 10 | 8 | 7 | 0 | c12cHcHcHcHc1COC3HCH(OH)C2(OH)-O--O3- | c12ccccc1C(=O)C3C(O)C2(O)OO3 | 0.533E-04 | 98.4 |
| **NaOOKK** | 192. | 10 | 8 | 4 | 0 | c12cHcHcHcHc1COCH(OH)COC2H(OH) | c12ccccc1C(=O)C(O)C(=O)C2(O) | 0.191E-06 | 122.3 |
| **NaOOKort** | 176. | 10 | 8 | 3 | 0 | c12cHcHcHcHc1CH(OH)COCdH=Cd2(OH) | c12ccccc1C(O)C(=O)C=C2(O) | 0.317E-05 | 109.7 |
| **NaOONBp** | 287. | 10 | 9 | 9 | 1 | c12cHcHcHcHc1CH(ONO2)C3HCH(OH)C2(OH)-O--O3- | c12ccccc1C(ON(=O)=O)C3C(O)C2(O)OO3 | 0.193E-05 | 114.4 |
| **NaOONort** | 223. | 10 | 9 | 5 | 1 | c12cHcHcHcHc1CH(OH)CH(ONO2)CdH=Cd2(OH) | c12ccccc1C(O)C(ON(=O)=O)C=C2(O) | 0.261E-06 | 122.2 |
| **NaOOO** | 176. | 10 | 8 | 3 | 0 | c12cHcHcHcHc1cHc(OH)c(OH)c2(OH) | c12ccccc1cc(O)c(O)c2(O) | 0.183E-09 | 152.4 |
| **NaOOOBp** | 242. | 10 | 10 | 7 | 0 | c12cHcHcHcHc1CH(OH)C3HCH(OH)C2(OH)-O--O3- | c12ccccc1C(O)C3C(O)C2(O)OO3 | 0.564E-05 | 110.9 |
| **NaOOOHBp** | 274. | 10 | 10 | 9 | 0 | c12cHcHcHcHc1C(OH)(OOH)C3HCH(OH)C2(OH)-O--O3- | c12ccccc1C(O)(OO)C3C(O)C2(O)OO3 | 0.346E-08 | 145.9 |
| **NaOOOK** | 194. | 10 | 10 | 4 | 0 | c12cHcHcHcHc1COCH(OH)CH(OH)C2H(OH) | c12ccccc1C(=O)C(O)C(O)C2(O) | 0.180E-07 | 134.9 |
| **NaOOONBp** | 303. | 10 | 9 | 10 | 1 | c12cHcHcHcHc1C(OH)(ONO2)C3HCH(OH)C2(OH)-O--O3- | c12ccccc1C(O)(ON(=O)=O)C3C(O)C2(O)OO3 | 0.284E-07 | 135.6 |
| **NaOOOOBp** | 258. | 10 | 10 | 8 | 0 | c12cHcHcHcHc1C(OH)(OH)C3HCH(OH)C2(OH)-O--O3- | c12ccccc1C(O)(O)C3C(O)C2(O)OO3 | 0.316E-04 | 103.7 |
| **NaOOOort** | 178. | 10 | 10 | 3 | 0 | c12cHcHcHcHc1CH(OH)CH(OH)CdH=Cd2(OH) | c12ccccc1C(O)C(O)C=C2(O) | 0.493E-06 | 120.3 |

| Name | MW (g mol$^{-1}$) | nbC | nbH | nbO | nbN | Chem code (GECKO-A) | Smile code | $P^{sat}$ (torr) | $\Delta H^{vap}$ (kJ) |
|---|---|---|---|---|---|---|---|---|---|
| **NaOOort** | 162. | 10 | 10 | 2 | 0 | c12cHcHcHcHc1CdH=CdHCH(OH)C2H(OH) | c12ccccc1C=CC(O)C2(O) | 0.371E-04 | 98.6 |
| **NaOOpar** | 162. | 10 | 10 | 2 | 0 | c12cHcHcHcHc1CH(OH)CdH=CdHC2H(OH) | c12ccccc1C(O)C=CC2(O) | 0.371E-04 | 98.6 |
| **NaOPEN** | 160. | 10 | 8 | 2 | 0 | CHOc1cHcHcHcHc1CdH=CdHCHO | C(=O)c1ccccc1C=CC=O | 0.271E-03 | 86.5 |
| **NaOPENOL** | 176. | 10 | 8 | 3 | 0 | CHOc1cHcHcHcHc1Cd(OH)=CdHCHO | C(=O)c1ccccc1C(O)=CC=O | 0.461E-05 | 107.0 |
| **NAPH** | 128. | 10 | 8 | 0 | 0 | c12cHcHcHcHc1cHcHcHc2H | c12ccccc1cccc2 | 0.503E-03 | 81.0 |
| **NaQuin** | 158. | 10 | 6 | 2 | 0 | c12cHcHcHcHc1COCdH=CdHC2O | c12ccccc1C(=O)C=CC2=O | 0.566E-02 | 70.9 |
| **NaV** | 173. | 10 | 7 | 2 | 1 | c12cHcHcHcHc1cHcHcHc2(NO2) | c12ccccc1cccc2(N(=O)=O) | 0.415E-05 | 102.8 |
| **NaVO** | 189. | 10 | 7 | 3 | 1 | c12cHcHcHcHc1cHcHc(OH)c2(NO2) | c12ccccc1ccc(O)c2(N(=O)=O) | 0.348E-07 | 126.1 |
| **NaVOO** | 205. | 10 | 7 | 4 | 1 | c12cHcHcHcHc1cHc(OH)c(NO2)c2(OH) | c12ccccc1cc(O)c(N(=O)=O)c2(O) | 0.176E-09 | 152.1 |
| **OHPhUA** | 196. | 9 | 8 | 5 | 0 | c1(OOH)cHcHcHc(OH)c1CdH=CdHCO(OH) | c1(OO)cccc(O)c1C=CC(=O)(O) | 0.528E-10 | 161.5 |
| **ONaHOOK** | 226. | 10 | 10 | 6 | 0 | c12cHcHcHc(OH)c1COCH(OH)CH(OOH)C2H(OH) | c12cccc(O)c1C(=O)C(O)C(OO)C2(O) | 0.212E-11 | 177.7 |
| **ONaNOOK** | 255. | 10 | 9 | 7 | 1 | c12cHcHcHc(OH)c1COCH(OH)CH(ONO2)C2H(OH) | c12cccc(O)c1C(=O)C(O)C(ON(=O)=O)C2(O) | 0.569E-10 | 161.7 |
| **ONaO** | 160. | 10 | 8 | 2 | 0 | c12cHcHcHc(OH)c1cHcHcHc2(OH) | c12cccc(O)c1cccc2(O) | 0.398E-07 | 125.8 |
| **ONaOHBp** | 258. | 10 | 10 | 8 | 0 | c12cHcHcHc(OH)c1CH(OOH)C3HCH(OH)C2H-O--O3- | c12cccc(O)c1C(OO)C3C(O)C2OO3 | 0.249E-06 | 123.3 |
| **ONaOHort** | 194. | 10 | 10 | 4 | 0 | c12cHcHcHc(OH)c1CdH=CdHCH(OOH)C2H(OH) | c12cccc(O)c1C=CC(OO)C2(O) | 0.147E-07 | 134.8 |
| **ONaOHpar** | 194. | 10 | 10 | 4 | 0 | c12cHcHcHc(OH)c1CH(OOH)CdH=CdHC2H(OH) | c12cccc(O)c1C(OO)C=CC2(O) | 0.147E-07 | 134.8 |
| **ONaOKBp** | 240. | 10 | 8 | 7 | 0 | c12cHcHcHc(OH)c1COC3HCH(OH)C2H-O--O3- | c12cccc(O)c1C(=O)C3C(O)C2OO3 | 0.434E-04 | 98.0 |
| **ONaOKort** | 176. | 10 | 8 | 3 | 0 | c12cHcHcHc(OH)c1CdH=CdHCOC2H(OH) | c12cccc(O)c1C=CC(=O)C2(O) | 0.225E-05 | 109.9 |
| **ONaOKpar** | 176. | 10 | 8 | 3 | 0 | c12cHcHcHc(OH)c1COCdH=CdHC2H(OH) | c12cccc(O)c1C(=O)C=CC2(O) | 0.357E-05 | 107.4 |
| **ONaONBp** | 287. | 10 | 9 | 9 | 1 | c12cHcHcHc(OH)c1CH(ONO2)C3HCH(OH)C2H-O--O3- | c12cccc(O)c1C(ON(=O)=O)C3C(O)C2OO3 | 0.165E-05 | 113.9 |
| **ONaONort** | 223. | 10 | 9 | 5 | 1 | c12cHcHcHc(OH)c1CdH=CdHCH(ONO2)C2H(OH) | c12cccc(O)c1C=CC(ON(=O)=O)C2(O) | 0.199E-06 | 122.1 |
| **ONaONpar** | 223. | 10 | 9 | 5 | 1 | c12cHcHcHc(OH)c1CH(ONO2)CdH=CdHC2H(OH) | c12cccc(O)c1C(ON(=O)=O)C=CC2(O) | 0.199E-06 | 122.1 |
| **ONaOOBp** | 242. | 10 | 10 | 7 | 0 | c12cHcHcHc(OH)c1CH(OH)C3HCH(OH)C2H-O--O3- | c12cccc(O)c1C(O)C3C(O)C2OO3 | 0.421E-05 | 110.9 |
| **ONaOOKK** | 208. | 10 | 8 | 5 | 0 | c12cHcHcHc(OH)c1COCH(OH)COC2H(OH) | c12cccc(O)c1C(=O)C(O)C(=O)C2(O) | 0.887E-09 | 147.9 |
| **ONaOOOK** | 210. | 10 | 10 | 5 | 0 | c12cHcHcHc(OH)c1COCH(OH)CH(OH)C2H(OH) | c12cccc(O)c1C(=O)C(O)C(O)C2(O) | 0.630E-10 | 161.8 |
| **ONaOOort** | 178. | 10 | 10 | 3 | 0 | c12cHcHcHc(OH)c1CdH=CdHCH(OH)C2H(OH) | c12cccc(O)c1C=CC(O)C2(O) | 0.308E-06 | 121.0 |
| **ONaOOpar** | 178. | 10 | 10 | 3 | 0 | c12cHcHcHc(OH)c1CH(OH)CdH=CdHC2H(OH) | c12cccc(O)c1C(O)C=CC2(O) | 0.308E-06 | 121.0 |
| **ONaOPEN** | 176. | 10 | 8 | 3 | 0 | CHOc1cHcHcHc(OH)c1CdH=CdHCHO | C(=O)c1cccc(O)c1C=CC=O | 0.348E-05 | 106.9 |
| **ONaQuin** | 174. | 10 | 6 | 3 | 0 | c12cHcHcHc(OH)c1COCdH=CdHC2O | c12cccc(O)c1C(=O)C=CC2=O | 0.526E-04 | 93.0 |

| Name | MW (g mol$^{-1}$) | nbC | nbH | nbO | nbN | Chem code (GECKO-A) | Smile code | $P^{sat}$ (torr) | $\Delta H^{vap}$ (kJ) |
|---|---|---|---|---|---|---|---|---|---|
| **OOPhUA** | 180. | 9 | 8 | 4 | 0 | c1(OH)cHcHcHc(OH)c1CdH=CdHCO(OH) | c1(O)cccc(O)c1C=CC(=O)(O) | 0.715E-08 | 137.8 |
| **OPh** | 94. | 6 | 6 | 1 | 0 | c1HcHcHcHcHc1(OH) | c1ccccc1(O) | 0.153E+01 | 50.9 |
| **OPhA** | 138. | 7 | 6 | 3 | 0 | CO(OH)c1cHcHcHcHc1(OH) | C(=O)(O)c1ccccc1(O) | 0.709E-04 | 95.7 |
| **OPhAD** | 166. | 8 | 6 | 4 | 0 | CHOc1cHcHcHc(OH)c1CO(OH) | C(=O)c1cccc(O)c1C(=O)(O) | 0.752E-06 | 115.6 |
| **OPhAUA** | 208. | 10 | 8 | 5 | 0 | CO(OH)c1cHcHcHc(OH)c1CdH=CdHCO(OH) | C(=O)(O)c1cccc(O)c1C=CC(=O)(O) | 0.538E-11 | 172.4 |
| **OPhD** | 122. | 7 | 6 | 2 | 0 | CHOc1cHcHcHc(OH)c1H | C(=O)c1cccc(O)c1 | 0.348E-01 | 66.3 |
| **OPhDCA** | 180. | 9 | 8 | 4 | 0 | CHOc1cHcHcHc(OH)c1CH2CO(OH) | C(=O)c1cccc(O)c1CC(=O)(O) | 0.327E-06 | 119.6 |
| **OPhDCD** | 164. | 9 | 8 | 3 | 0 | CHOc1cHcHcHc(OH)c1CH2CHO | C(=O)c1cccc(O)c1CC=O | 0.624E-04 | 94.3 |
| **OPhDD** | 150. | 8 | 6 | 3 | 0 | CHOc1cHcHcHc(OH)c1CHO | C(=O)c1cccc(O)c1C=O | 0.144E-03 | 90.0 |
| **OPhDHOD** | 226. | 10 | 10 | 6 | 0 | CHOc1cHcHcHc(OH)c1CH(OOH)CH(OH)CHO | C(=O)c1cccc(O)c1C(OO)C(O)C=O | 0.457E-10 | 162.1 |
| **OPhDKOD** | 208. | 10 | 8 | 5 | 0 | CHOc1cHcHcHc(OH)c1COCH(OH)CHO | C(=O)c1cccc(O)c1C(=O)C(O)C=O | 0.347E-07 | 129.4 |
| **OPhDNOD** | 255. | 10 | 9 | 7 | 1 | CHOc1cHcHcHc(OH)c1CH(ONO2)CH(OH)CHO | C(=O)c1cccc(O)c1C(ON(=O)=O)C(O)C=O | 0.779E-09 | 148.4 |
| **OPhDOOD** | 210. | 10 | 10 | 5 | 0 | CHOc1cHcHcHc(OH)c1CH(OH)CH(OH)CHO | C(=O)c1cccc(O)c1C(O)C(O)C=O | 0.110E-08 | 147.3 |
| **OPhKA** | 166. | 8 | 6 | 4 | 0 | c1(OH)cHcHcHcHc1COCO(OH) | c1(O)ccccc1C(=O)C(=O)(O) | 0.267E-05 | 109.8 |
| **OPhKKA** | 194. | 9 | 6 | 5 | 0 | c1(OH)cHcHcHcHc1COCOCO(OH) | c1(O)ccccc1C(=O)C(=O)C(=O)(O) | 0.420E-07 | 128.8 |
| **OPhKOA** | 196. | 9 | 8 | 5 | 0 | c1(OH)cHcHcHcHc1COCH(OH)CO(OH) | c1(O)ccccc1C(=O)C(O)C(=O)(O) | 0.266E-08 | 143.2 |
| **OPhOA** | 168. | 8 | 8 | 4 | 0 | c1(OH)cHcHcHcHc1CH(OH)CO(OH) | c1(O)ccccc1C(O)C(=O)(O) | 0.122E-06 | 126.1 |
| **OPhODKD** | 208. | 10 | 8 | 5 | 0 | CHOCOc1cHcHcHc(OH)c1CH(OH)CHO | O=CC(=O)c1cccc(O)c1C(O)C=O | 0.280E-07 | 130.6 |
| **OPhOUA** | 180. | 9 | 8 | 4 | 0 | c1(OH)cHcHcHcHc1Cd(OH)=CdHCO(OH) | c1(O)ccccc1C(O)=CC(=O)(O) | 0.109E-07 | 137.1 |
| **OPhUA** | 164. | 9 | 8 | 3 | 0 | c1(OH)cHcHcHcHc1CdH=CdHCO(OH) | c1(O)ccccc1C=CC(=O)(O) | 0.118E-05 | 113.8 |
| **OPhUAnhy** | 190. | 10 | 6 | 4 | 0 | c12cHcHcHc(OH)c1CdH=CdHCO-O-C2O | c12cccc(O)c1C=CC(=O)OC2=O | 0.147E-07 | 130.8 |
| **PhA** | 122. | 7 | 6 | 2 | 0 | c1HcHcHcHcHc1CO(OH) | c1ccccc1C(=O)(O) | 0.892E-02 | 74.1 |
| **PhAA** | 166. | 8 | 6 | 4 | 0 | CO(OH)c1cHcHcHcHc1CO(OH) | C(=O)(O)c1ccccc1C(=O)(O) | 0.471E-06 | 117.6 |
| **PhAD** | 150. | 8 | 6 | 3 | 0 | CHOc1cHcHcHcHc1CO(OH) | C(=O)c1ccccc1C(=O)(O) | 0.117E-03 | 92.3 |
| **PhAKD** | 178. | 9 | 6 | 4 | 0 | CHOCOc1cHcHcHcHc1CO(OH) | O=CC(=O)c1ccccc1C(=O)(O) | 0.397E-05 | 107.3 |
| **PhAKOA** | 224. | 10 | 8 | 6 | 0 | CO(OH)c1cHcHcHcHc1COCH(OH)CO(OH) | C(=O)(O)c1ccccc1C(=O)C(O)C(=O)(O) | 0.145E-11 | 179.5 |
| **PhAKOD** | 208. | 10 | 8 | 5 | 0 | CO(OH)c1cHcHcHcHc1COCH(OH)CHO | C(=O)(O)c1ccccc1C(=O)C(O)C=O | 0.414E-08 | 140.5 |
| **PhAND** | 225. | 9 | 7 | 6 | 1 | CO(OH)c1cHcHcHcHc1CH(ONO2)CHO | C(=O)(O)c1ccccc1C(ON(=O)=O)C=O | 0.119E-06 | 124.7 |
| **PhAnhy** | 148. | 8 | 4 | 3 | 0 | c12cHcHcHcHc1CO-O-C2O | c12ccccc1C(=O)OC2=O | 0.153E-04 | 97.6 |

| Name | MW (g mol$^{-1}$) | nbC | nbH | nbO | nbN | Chem code (GECKO-A) | Smile code | $P^{sat}$ (torr) | $\Delta H^{vap}$ (kJ) |
|---|---|---|---|---|---|---|---|---|---|
| **PhAOCA** | 210. | 10 | 10 | 5 | 0 | CO(OH)c1cHcHcHcHc1CH(OH)CH2CO(OH) | C(=O)(O)c1ccccc1C(O)CC(=O)(O) | 0.294E-10 | 165.3 |
| **PhAOCD** | 194. | 10 | 10 | 4 | 0 | CO(OH)c1cHcHcHcHc1CH(OH)CH2CHO | C(=O)(O)c1ccccc1C(O)CC=O | 0.426E-07 | 130.0 |
| **PhAOCG** | 226. | 10 | 10 | 6 | 0 | CO(OH)c1cHcHcHcHc1CH(OH)CH2CO(OOH) | C(=O)(O)c1ccccc1C(O)CC(=O)(OO) | 0.249E-09 | 155.2 |
| **PhAOCP** | 271. | 10 | 9 | 8 | 1 | CO(OH)c1cHcHcHcHc1CH(OH)CH2CO(OONO2) | C(=O)(O)c1ccccc1C(O)CC(=O)(OON(=O)=O) | 0.233E-08 | 143.9 |
| **PhAOD** | 180. | 9 | 8 | 4 | 0 | CO(OH)c1cHcHcHcHc1CH(OH)CHO | C(=O)(O)c1ccccc1C(O)C=O | 0.136E-06 | 124.8 |
| **PhAOH** | 198. | 9 | 10 | 5 | 0 | CO(OH)c1cHcHcHcHc1CH(OH)CH2(OOH) | C(=O)(O)c1ccccc1C(O)C(OO) | 0.227E-09 | 155.6 |
| **PhAOKA** | 224. | 10 | 8 | 6 | 0 | CO(OH)CH(OH)c1cHcHcHcHc1COCO(OH) | C(=O)(O)C(O)c1ccccc1C(=O)C(=O)(O) | 0.145E-11 | 179.5 |
| **PhAOKD** | 208. | 10 | 8 | 5 | 0 | CHOCOc1cHcHcHcHc1CH(OH)CO(OH) | O=CC(=O)c1ccccc1C(O)C(=O)(O) | 0.414E-08 | 140.5 |
| **PhAON** | 227. | 9 | 9 | 6 | 1 | CO(OH)c1cHcHcHcHc1CH(OH)CH2(ONO2) | C(=O)(O)c1ccccc1C(O)C(ON(=O)=O) | 0.430E-08 | 141.5 |
| **PhAOO** | 182. | 9 | 10 | 4 | 0 | CO(OH)c1cHcHcHcHc1CH(OH)CH2(OH) | C(=O)(O)c1ccccc1C(O)C(O) | 0.402E-08 | 142.1 |
| **PhAOOA** | 212. | 9 | 8 | 6 | 0 | CO(OH)c1cHcHcHcHc1C(OH)(OH)CO(OH) | C(=O)(O)c1ccccc1C(O)(O)C(=O)(O) | 0.131E-08 | 148.0 |
| **PhAOUA** | 208. | 10 | 8 | 5 | 0 | CO(OH)c1cHcHcHcHc1Cd(OH)=CdHCO(OH) | C(=O)(O)c1ccccc1C(O)=CC(=O)(O) | 0.758E-11 | 171.7 |
| **PhAOUD** | 192. | 10 | 8 | 4 | 0 | CO(OH)c1cHcHcHcHc1Cd(OH)=CdHCHO | C(=O)(O)c1ccccc1C(O)=CC=O | 0.131E-07 | 135.5 |
| **PhAUA** | 192. | 10 | 8 | 4 | 0 | CO(OH)c1cHcHcHcHc1CdH=CdHCO(OH) | C(=O)(O)c1ccccc1C=CC(=O)(O) | 0.566E-08 | 138.1 |
| **PhAUD1** | 176. | 10 | 8 | 3 | 0 | CO(OH)c1cHcHcHcHc1CdH=CdHCHO | C(=O)(O)c1ccccc1C=CC=O | 0.189E-05 | 110.8 |
| **PhAUD2** | 176. | 10 | 8 | 3 | 0 | CHOc1cHcHcHcHc1CdH=CdHCO(OH) | C(=O)c1ccccc1C=CC(=O)(O) | 0.227E-05 | 109.8 |
| **PhD** | 106. | 7 | 6 | 1 | 0 | c1HcHcHcHcHc1CHO | c1ccccc1C=O | 0.144E+01 | 49.7 |
| **PhDCA** | 164. | 9 | 8 | 3 | 0 | CHOc1cHcHcHcHc1CH2CO(OH) | C(=O)c1ccccc1CC(=O)(O) | 0.501E-04 | 96.3 |
| **PhDCD** | 148. | 9 | 8 | 2 | 0 | CHOc1cHcHcHcHc1CH2CHO | C(=O)c1ccccc1CC=O | 0.386E-02 | 75.3 |
| **PhDD** | 134. | 8 | 6 | 2 | 0 | CHOc1cHcHcHcHc1CHO | C(=O)c1ccccc1C=O | 0.842E-02 | 71.3 |
| **PhDHOD** | 210. | 10 | 10 | 5 | 0 | CHOc1cHcHcHcHc1CH(OOH)CH(OH)CHO | C(=O)c1ccccc1C(OO)C(O)C=O | 0.854E-08 | 137.1 |
| **PhDKA** | 178. | 9 | 6 | 4 | 0 | CHOc1cHcHcHcHc1COCO(OH) | C(=O)c1ccccc1C(=O)C(=O)(O) | 0.473E-05 | 106.2 |
| **PhDKHD** | 208. | 10 | 8 | 5 | 0 | CHOc1cHcHcHcHc1COCH(OOH)CHO | C(=O)c1ccccc1C(=O)C(OO)C=O | 0.288E-06 | 118.9 |
| **PhDKKD** | 190. | 10 | 6 | 4 | 0 | CHOc1cHcHcHcHc1COCOCHO | C(=O)c1ccccc1C(=O)C(=O)C=O | 0.429E-04 | 94.4 |
| **PhDKND** | 237. | 10 | 7 | 6 | 1 | CHOc1cHcHcHcHc1COCH(ONO2)CHO | C(=O)c1ccccc1C(=O)C(ON(=O)=O)C=O | 0.272E-05 | 108.0 |
| **PhDKOD** | 192. | 10 | 8 | 4 | 0 | CHOc1cHcHcHcHc1COCH(OH)CHO | C(=O)c1ccccc1C(=O)C(O)C=O | 0.438E-05 | 106.6 |
| **PhDNOD** | 239. | 10 | 9 | 6 | 1 | CHOc1cHcHcHcHc1CH(ONO2)CH(OH)CHO | C(=O)c1ccccc1C(ON(=O)=O)C(O)C=O | 0.607E-07 | 127.7 |
| **PhDOOD** | 194. | 10 | 10 | 4 | 0 | CHOc1cHcHcHcHc1CH(OH)CH(OH)CHO | C(=O)c1ccccc1C(O)C(O)C=O | 0.166E-06 | 123.6 |
| **PhDOOD1** | 180. | 9 | 8 | 4 | 0 | CHOc1cHcHcHcHc1C(OH)(OH)CHO | C(=O)c1ccccc1C(O)(O)C=O | 0.229E-03 | 90.0 |

| Name | MW (g mol$^{-1}$) | nbC | nbH | nbO | nbN | Chem code (GECKO-A) | Smile code | $P^{sat}$ (torr) | $\Delta H^{vap}$ (kJ) |
|---|---|---|---|---|---|---|---|---|---|
| **PhDOOHD** | 226. | 10 | 10 | 6 | 0 | CHOc1cHcHcHcHc1C(OH)(OH)CH(OOH)CHO | C(=O)c1ccccc1C(O)(O)C(OO)C=O | 0.731E-07 | 127.5 |
| **PhDOOKD** | 208. | 10 | 8 | 5 | 0 | CHOc1cHcHcHcHc1C(OH)(OH)COCHO | C(=O)c1ccccc1C(O)(O)C(=O)C=O | 0.165E-04 | 101.3 |
| **PhDOOND** | 255. | 10 | 9 | 7 | 1 | CHOc1cHcHcHcHc1C(OH)(OH)CH(ONO2)CHO | C(=O)c1ccccc1C(O)(O)C(ON(=O)=O)C=O | 0.396E-06 | 119.4 |
| **PhDOOOD** | 210. | 10 | 10 | 5 | 0 | CHOc1cHcHcHcHc1C(OH)(OH)CH(OH)CHO | C(=O)c1ccccc1C(O)(O)C(O)C=O | 0.128E-05 | 114.7 |
| **PhEstH** | 166. | 8 | 6 | 4 | 0 | c12cHcHcHcHc1CO-O-C2H(OOH) | c12ccccc1C(=O)OC2(OO) | 0.702E-05 | 102.4 |
| **PhEstO** | 150. | 8 | 6 | 3 | 0 | c12cHcHcHcHc1CO-O-C2H(OH) | c12ccccc1C(=O)OC2(O) | 0.988E-04 | 90.4 |
| **PhGA** | 182. | 8 | 6 | 5 | 0 | CO(OH)c1cHcHcHcHc1CO(OOH) | C(=O)(O)c1ccccc1C(=O)(OO) | 0.255E-05 | 109.9 |
| **PhGD** | 166. | 8 | 6 | 4 | 0 | CHOc1cHcHcHcHc1CO(OOH) | C(=O)c1ccccc1C(=O)(OO) | 0.492E-03 | 85.7 |
| **PhGKOA** | 240. | 10 | 8 | 7 | 0 | CO(OH)c1cHcHcHcHc1COCH(OH)CO(OOH) | C(=O)(O)c1ccccc1C(=O)C(O)C(=O)(OO) | 0.137E-10 | 168.7 |
| **PhGKOD** | 224. | 10 | 8 | 6 | 0 | CO(OOH)c1cHcHcHcHc1COCH(OH)CHO | C(=O)(OO)c1ccccc1C(=O)C(O)C=O | 0.262E-07 | 131.8 |
| **PhGND** | 241. | 9 | 7 | 7 | 1 | CO(OOH)c1cHcHcHcHc1CH(ONO2)CHO | C(=O)(OO)c1ccccc1C(ON(=O)=O)C=O | 0.577E-06 | 117.2 |
| **PhGOCD** | 210. | 10 | 10 | 5 | 0 | CO(OOH)c1cHcHcHcHc1CH(OH)CH2CHO | C(=O)(OO)c1ccccc1C(O)CC=O | 0.254E-06 | 121.7 |
| **PhGOKA** | 240. | 10 | 8 | 7 | 0 | CO(OH)CH(OH)c1cHcHcHcHc1COCO(OOH) | C(=O)(O)C(O)c1ccccc1C(=O)C(=O)(OO) | 0.137E-10 | 168.7 |
| **PhGOKD** | 224. | 10 | 8 | 6 | 0 | CHOCOc1cHcHcHcHc1CH(OH)CO(OOH) | O=CC(=O)c1ccccc1C(O)C(=O)(OO) | 0.262E-07 | 131.8 |
| **PhGOUA** | 224. | 10 | 8 | 6 | 0 | CO(OH)c1cHcHcHcHc1Cd(OH)=CdHCO(OOH) | C(=O)(O)c1ccccc1C(O)=CC(=O)(OO) | 0.703E-10 | 161.1 |
| **PhGOUD** | 208. | 10 | 8 | 5 | 0 | CO(OOH)c1cHcHcHcHc1Cd(OH)=CdHCHO | C(=O)(OO)c1ccccc1C(O)=CC=O | 0.846E-07 | 126.8 |
| **PhGUA1** | 208. | 10 | 8 | 5 | 0 | CO(OH)c1cHcHcHcHc1CdH=CdHCO(OOH) | C(=O)(O)c1ccccc1C=CC(=O)(OO) | 0.360E-07 | 129.4 |
| **PhGUA2** | 208. | 10 | 8 | 5 | 0 | CO(OOH)c1cHcHcHcHc1CdH=CdHCO(OH) | C(=O)(OO)c1ccccc1C=CC(=O)(O) | 0.360E-07 | 129.4 |
| **PhGUD1** | 192. | 10 | 8 | 4 | 0 | CO(OOH)c1cHcHcHcHc1CdH=CdHCHO | C(=O)(OO)c1ccccc1C=CC=O | 0.943E-05 | 103.4 |
| **PhGUD2** | 192. | 10 | 8 | 4 | 0 | CHOc1cHcHcHcHc1CdH=CdHCO(OOH) | C(=O)c1ccccc1C=CC(=O)(OO) | 0.112E-04 | 102.3 |
| **PhKA** | 150. | 8 | 6 | 3 | 0 | c1HcHcHcHcHc1COCO(OH) | c1ccccc1C(=O)C(=O)(O) | 0.404E-03 | 86.4 |
| **PhKAKA** | 222. | 10 | 6 | 6 | 0 | CO(OH)COc1cHcHcHcHc1COCO(OH) | C(=O)(O)C(=O)c1ccccc1C(=O)C(=O)(O) | 0.631E-10 | 160.0 |
| **PhKAnhy** | 176. | 9 | 4 | 4 | 0 | c12cHcHcHcHc1COCO-O-C2O | c12ccccc1C(=O)C(=O)OC2=O | 0.625E-06 | 112.4 |
| **PhKD** | 134. | 8 | 6 | 2 | 0 | c1HcHcHcHcHc1COCHO | c1ccccc1C(=O)C=O | 0.107E+00 | 60.7 |
| **PhKDD** | 162. | 9 | 6 | 3 | 0 | CHOCOc1cHcHcHcHc1CHO | O=CC(=O)c1ccccc1C=O | 0.128E-02 | 79.2 |
| **PhKDKD** | 190. | 10 | 6 | 4 | 0 | CHOCOc1cHcHcHcHc1COCHO | O=CC(=O)c1ccccc1C(=O)C=O | 0.551E-04 | 93.2 |
| **PhKG** | 166. | 8 | 6 | 4 | 0 | c1HcHcHcHcHc1COCO(OOH) | c1ccccc1C(=O)C(=O)(OO) | 0.149E-02 | 80.4 |
| **PhKKAnhy** | 204. | 10 | 4 | 5 | 0 | c12cHcHcHcHc1COCO-O-COC2O | c12ccccc1C(=O)C(=O)OC(=O)C2=O | 0.786E-07 | 121.8 |
| **PhKOA** | 180. | 9 | 8 | 4 | 0 | c1HcHcHcHcHc1COCH(OH)CO(OH) | c1ccccc1C(=O)C(O)C(=O)(O) | 0.574E-06 | 117.9 |

| Name | MW (g mol$^{-1}$) | nbC | nbH | nbO | nbN | Chem code (GECKO-A) | Smile code | $P^{sat}$ (torr) | $\Delta H^{vap}$ (kJ) |
|---|---|---|---|---|---|---|---|---|---|
| **PhKOAnhy** | 206. | 10 | 6 | 5 | 0 | c12cHcHcHcHc1COCH(OH)CO-O-C2O | c12ccccc1C(=O)C(O)C(=O)OC2=O | 0.174E-08 | 141.5 |
| **PhKOG** | 196. | 9 | 8 | 5 | 0 | c1HcHcHcHcHc1COCH(OH)CO(OOH) | c1ccccc1C(=O)C(O)C(=O)(OO) | 0.300E-05 | 110.3 |
| **PhKOHEst** | 224. | 10 | 8 | 6 | 0 | c12cHcHcHcHc1COCH(OH)CH(OOH)-O-C2O | c12ccccc1C(=O)C(O)C(OO)OC2=O | 0.132E-09 | 155.6 |
| **PhKOOEst** | 208. | 10 | 8 | 5 | 0 | c12cHcHcHcHc1COCH(OH)CH(OH)-O-C2O | c12ccccc1C(=O)C(O)C(O)OC2=O | 0.274E-08 | 141.3 |
| **PhKOP** | 241. | 9 | 7 | 7 | 1 | c1HcHcHcHcHc1COCH(OH)CO(OONO2) | c1ccccc1C(=O)C(O)C(=O)(OON(=O)=O) | 0.218E-04 | 99.6 |
| **PhKP** | 211. | 8 | 5 | 6 | 1 | c1HcHcHcHcHc1COCO(OONO2) | c1ccccc1C(=O)C(=O)(OON(=O)=O) | 0.338E-02 | 75.6 |
| **PhNA** | 197. | 8 | 7 | 5 | 1 | c1HcHcHcHcHc1CH(ONO2)CO(OH) | c1ccccc1C(ON(=O)=O)C(=O)(O) | 0.124E-04 | 103.9 |
| **PhNDKD** | 237. | 10 | 7 | 6 | 1 | CHOCOc1cHcHcHcHc1CH(ONO2)CHO | O=CC(=O)c1ccccc1C(ON(=O)=O)C=O | 0.223E-05 | 109.2 |
| **PhNG** | 213. | 8 | 7 | 6 | 1 | c1HcHcHcHcHc1CH(ONO2)CO(OOH) | c1ccccc1C(ON(=O)=O)C(=O)(OO) | 0.494E-04 | 97.4 |
| **PhNP** | 258. | 8 | 6 | 8 | 2 | c1HcHcHcHcHc1CH(ONO2)CO(OONO2) | c1ccccc1C(ON(=O)=O)C(=O)(OON(=O)=O) | 0.186E-03 | 89.9 |
| **PhOA** | 152. | 8 | 8 | 3 | 0 | c1HcHcHcHcHc1CH(OH)CO(OH) | c1ccccc1C(O)C(=O)(O) | 0.182E-04 | 103.1 |
| **PhOCA** | 166. | 9 | 10 | 3 | 0 | c1HcHcHcHcHc1CH(OH)CH2CO(OH) | c1ccccc1C(O)CC(=O)(O) | 0.565E-05 | 108.2 |
| **PhOCAnhy** | 192. | 10 | 8 | 4 | 0 | c12cHcHcHcHc1CH(OH)CH2CO-O-C2O | c12ccccc1C(O)CC(=O)OC2=O | 0.129E-07 | 132.3 |
| **PhOCG** | 182. | 9 | 10 | 4 | 0 | c1HcHcHcHcHc1CH(OH)CH2CO(OOH) | c1ccccc1C(O)CC(=O)(OO) | 0.277E-04 | 100.9 |
| **PhOCHEst** | 210. | 10 | 10 | 5 | 0 | c12cHcHcHcHc1CH(OH)CH2CH(OOH)-O-C2O | c12ccccc1C(O)CC(OO)OC2=O | 0.263E-08 | 141.3 |
| **PhOCOEst** | 194. | 10 | 10 | 4 | 0 | c12cHcHcHcHc1CH(OH)CH2CH(OH)-O-C2O | c12ccccc1C(O)CC(O)OC2=O | 0.507E-07 | 127.5 |
| **PhOCP** | 227. | 9 | 9 | 6 | 1 | c1HcHcHcHcHc1CH(OH)CH2CO(OONO2) | c1ccccc1C(O)CC(=O)(OON(=O)=O) | 0.146E-03 | 92.0 |
| **PhOD** | 136. | 8 | 8 | 2 | 0 | c1HcHcHcHcHc1CH(OH)CHO | c1ccccc1C(O)C=O | 0.956E-02 | 73.7 |
| **PhODKD** | 192. | 10 | 8 | 4 | 0 | CHOCOc1cHcHcHcHc1CH(OH)CHO | O=CC(=O)c1ccccc1C(O)C=O | 0.366E-05 | 107.7 |
| **PhOG** | 168. | 8 | 8 | 4 | 0 | c1HcHcHcHcHc1CH(OH)CO(OOH) | c1ccccc1C(O)C(=O)(OO) | 0.889E-04 | 95.9 |
| **PhOH** | 154. | 8 | 10 | 3 | 0 | c1HcHcHcHcHc1CH(OH)CH2(OOH) | c1ccccc1C(O)C(OO) | 0.428E-04 | 98.3 |
| **PhOKAnhy** | 206. | 10 | 6 | 5 | 0 | c12cHcHcHcHc1COCO-O-COC2H(OH) | c12ccccc1C(=O)C(=O)OC(=O)C2(O) | 0.174E-08 | 141.5 |
| **PhOKHEst** | 224. | 10 | 8 | 6 | 0 | c12cHcHcHcHc1COCH(OOH)-O-COC2H(OH) | c12ccccc1C(=O)C(OO)OC(=O)C2(O) | 0.132E-09 | 155.6 |
| **PhOKOEst** | 208. | 10 | 8 | 5 | 0 | c12cHcHcHcHc1COCH(OH)-O-COC2H(OH) | c12ccccc1C(=O)C(O)OC(=O)C2(O) | 0.274E-08 | 141.3 |
| **PhON** | 183. | 8 | 9 | 4 | 1 | c1HcHcHcHcHc1CH(OH)CH2(ONO2) | c1ccccc1C(O)C(ON(=O)=O) | 0.405E-03 | 88.3 |
| **PhOO** | 138. | 8 | 10 | 2 | 0 | c1HcHcHcHcHc1CH(OH)CH2(OH) | c1ccccc1C(O)C(O) | 0.489E-03 | 87.4 |
| **PhOOAnhy** | 194. | 9 | 6 | 5 | 0 | c12cHcHcHcHc1C(OH)(OH)CO-O-C2O | c12ccccc1C(O)(O)C(=O)OC2=O | 0.326E-06 | 117.5 |
| **PhOP** | 213. | 8 | 7 | 6 | 1 | c1HcHcHcHcHc1CH(OH)CO(OONO2) | c1ccccc1C(O)C(=O)(OON(=O)=O) | 0.438E-03 | 87.3 |
| **PhOUA** | 164. | 9 | 8 | 3 | 0 | c1HcHcHcHcHc1Cd(OH)=CdHCO(OH) | c1ccccc1C(O)=CC(=O)(O) | 0.186E-05 | 113.2 |

| Name | MW (g mol$^{-1}$) | nbC | nbH | nbO | nbN | Chem code (GECKO-A) | Smile code | $P^{sat}$ (torr) | $\Delta H^{vap}$ (kJ) |
|---|---|---|---|---|---|---|---|---|---|
| **PhOUAnhy** | 190. | 10 | 6 | 4 | 0 | c12cHcHcHcHc1Cd(OH)=CdHCO-O-C2O | c12ccccc1C(O)=CC(=O)OC2=O | 0.152E-07 | 131.5 |
| **PhOUG** | 180. | 9 | 8 | 4 | 0 | c1HcHcHcHcHc1Cd(OH)=CdHCO(OOH) | c1ccccc1C(O)=CC(=O)(OO) | 0.993E-05 | 105.5 |
| **PhOUHEst** | 208. | 10 | 8 | 5 | 0 | c12cHcHcHcHc1Cd(OH)=CdHCH(OOH)-O-C2O | c12ccccc1C(O)=CC(OO)OC2=O | 0.447E-08 | 138.9 |
| **PhOUOEst** | 192. | 10 | 8 | 4 | 0 | c12cHcHcHcHc1Cd(OH)=CdHCH(OH)-O-C2O | c12ccccc1C(O)=CC(O)OC2=O | 0.856E-07 | 125.3 |
| **PhOUP** | 225. | 9 | 7 | 6 | 1 | c1HcHcHcHcHc1Cd(OH)=CdHCO(OONO2) | c1ccccc1C(O)=CC(=O)(OON(=O)=O) | 0.604E-04 | 96.0 |
| **PhPA** | 227. | 8 | 5 | 7 | 1 | CO(OH)c1cHcHcHcHc1CO(OONO2) | C(=O)(O)c1ccccc1C(=O)(OON(=O)=O) | 0.572E-05 | 106.5 |
| **PhPD** | 211. | 8 | 5 | 6 | 1 | CHOc1cHcHcHcHc1CO(OONO2) | C(=O)c1ccccc1C(=O)(OON(=O)=O) | 0.190E-02 | 78.1 |
| **PhPKOA** | 285. | 10 | 7 | 9 | 1 | CO(OH)c1cHcHcHcHc1COCH(OH)CO(OONO2) | C(=O)(O)c1ccccc1C(=O)C(O)C(=O)(OON(=O)=O | 0.212E-09 | 154.8 |
| **PhPKOD** | 269. | 10 | 7 | 8 | 1 | CO(OONO2)c1cHcHcHcHc1COCH(OH)CHO | C(=O)(OON(=O)=O)c1ccccc1C(=O)C(O)C=O | 0.253E-06 | 120.2 |
| **PhPND** | 286. | 9 | 6 | 9 | 2 | CO(OONO2)c1cHcHcHcHc1CH(ONO2)CHO | C(=O)(OON(=O)=O)c1ccccc1C(ON(=O)=O)C=O | 0.337E-05 | 107.8 |
| **PhPOCD** | 255. | 10 | 9 | 7 | 1 | CO(OONO2)c1cHcHcHcHc1CH(OH)CH2CHO | C(=O)(OON(=O)=O)c1ccccc1C(O)CC=O | 0.210E-05 | 110.8 |
| **PhPOKA** | 285. | 10 | 7 | 9 | 1 | CO(OH)CH(OH)c1cHcHcHcHc1COCO(OONO2) | C(=O)(O)C(O)c1ccccc1C(=O)C(=O)(OON(=O)=O | 0.212E-09 | 154.8 |
| **PhPOKD** | 269. | 10 | 7 | 8 | 1 | CHOCOc1cHcHcHcHc1CH(OH)CO(OONO2) | O=CC(=O)c1ccccc1C(O)C(=O)(OON(=O)=O) | 0.253E-06 | 120.2 |
| **PhPOUA** | 269. | 10 | 7 | 8 | 1 | CO(OH)c1cHcHcHcHc1Cd(OH)=CdHCO(OONO2) | C(=O)(O)c1ccccc1C(O)=CC(=O)(OON(=O)=O) | 0.758E-09 | 149.2 |
| **PhPOUD** | 253. | 10 | 7 | 7 | 1 | CO(OONO2)c1cHcHcHcHc1Cd(OH)=CdHCHO | C(=O)(OON(=O)=O)c1ccccc1C(O)=CC=O | 0.806E-06 | 115.2 |
| **PhPUA1** | 253. | 10 | 7 | 7 | 1 | CO(OH)c1cHcHcHcHc1CdH=CdHCO(OONO2) | C(=O)(O)c1ccccc1C=CC(=O)(OON(=O)=O) | 0.115E-06 | 124.1 |
| **PhPUA2** | 253. | 10 | 7 | 7 | 1 | CO(OONO2)c1cHcHcHcHc1CdH=CdHCO(OH) | C(=O)(OON(=O)=O)c1ccccc1C=CC(=O)(O) | 0.115E-06 | 124.1 |
| **PhPUD1** | 237. | 10 | 7 | 6 | 1 | CO(OONO2)c1cHcHcHcHc1CdH=CdHCHO | C(=O)(OON(=O)=O)c1ccccc1C=CC=O | 0.541E-04 | 94.1 |
| **PhPUD2** | 237. | 10 | 7 | 6 | 1 | CHOc1cHcHcHcHc1CdH=CdHCO(OONO2) | C(=O)c1ccccc1C=CC(=O)(OON(=O)=O) | 0.645E-04 | 93.0 |
| **PhUA** | 148. | 9 | 8 | 2 | 0 | c1HcHcHcHcHc1CdH=CdHCO(OH) | c1ccccc1C=CC(=O)(O) | 0.176E-03 | 90.7 |
| **PhUAnhy** | 174. | 10 | 6 | 3 | 0 | c12cHcHcHcHc1CdH=CdHCO-O-C2O | c12ccccc1C=CC(=O)OC2=O | 0.195E-05 | 107.0 |
| **PhUG** | 164. | 9 | 8 | 3 | 0 | c1HcHcHcHcHc1CdH=CdHCO(OOH) | c1ccccc1C=CC(=O)(OO) | 0.718E-03 | 84.3 |
| **PhUHEst1** | 192. | 10 | 8 | 4 | 0 | c12cHcHcHcHc1CdH=CdHCH(OOH)-O-C2O | c12ccccc1C=CC(OO)OC2=O | 0.945E-06 | 111.7 |
| **PhUHEst2** | 192. | 10 | 8 | 4 | 0 | c12cHcHcHcHc1CdH=CdHCO-O-C2H(OOH) | c12ccccc1C=CC(=O)OC2(OO) | 0.694E-06 | 113.0 |
| **PhUOEst1** | 176. | 10 | 8 | 3 | 0 | c12cHcHcHcHc1CdH=CdHCH(OH)-O-C2O | c12ccccc1C=CC(O)OC2=O | 0.132E-04 | 99.6 |
| **PhUOEst2** | 176. | 10 | 8 | 3 | 0 | c12cHcHcHcHc1CdH=CdHCO-O-C2H(OH) | c12ccccc1C=CC(=O)OC2(O) | 0.974E-05 | 100.8 |
| **PhUP** | 209. | 9 | 7 | 5 | 1 | c1HcHcHcHcHc1CdH=CdHCO(OONO2) | c1ccccc1C=CC(=O)(OON(=O)=O) | 0.257E-02 | 77.0 |
| **VOOPhUA** | 225. | 9 | 7 | 6 | 1 | c1(OH)c(NO2)cHcHc(OH)c1CdH=CdHCO(OH) | c1(O)c(N(=O)=O)ccc(O)c1C=CC(=O)(O) | 0.135E-10 | 167.2 |
| **VOPh** | 139. | 6 | 5 | 3 | 1 | c1HcHcHcHc(NO2)c1(OH) | c1cccc(N(=O)=O)c1(O) | 0.805E-02 | 72.1 |

| Name | MW (g mol$^{-1}$) | nbC | nbH | nbO | nbN | Chem code (GECKO-A) | Smile code | $P^{sat}$ (torr) | $\Delta H^{vap}$ (kJ) |
|---|---|---|---|---|---|---|---|---|---|
| **VOPhA** | 183. | 7 | 5 | 5 | 1 | CO(OH)c1cHcHcHc(OH)c1(NO2) | C(=O)(O)c1cccc(O)c1(N(=O)=O) | 0.201E-06 | 121.5 |
| **VOPhD** | 167. | 7 | 5 | 4 | 1 | CHOc1cHcHcHc(OH)c1(NO2) | C(=O)c1cccc(O)c1(N(=O)=O) | 0.187E-03 | 88.4 |
| **VOPhKA** | 211. | 8 | 5 | 6 | 1 | c1(OH)c(NO2)cHcHcHc1COCO(OH) | c1(O)c(N(=O)=O)cccc1C(=O)C(=O)(O) | 0.712E-08 | 136.7 |
| **VOPhKKA** | 239. | 9 | 5 | 7 | 1 | c1(OH)c(NO2)cHcHcHc1COCOCO(OH) | c1(O)c(N(=O)=O)cccc1C(=O)C(=O)C(=O)(O) | 0.979E-10 | 157.1 |
| **VOPhKOA** | 241. | 9 | 7 | 7 | 1 | c1(OH)c(NO2)cHcHcHc1COCH(OH)CO(OH) | c1(O)c(N(=O)=O)cccc1C(=O)C(O)C(=O)(O) | 0.409E-11 | 173.6 |
| **VOPhOA** | 213. | 8 | 7 | 6 | 1 | c1(OH)c(NO2)cHcHcHc1CH(OH)CO(OH) | c1(O)c(N(=O)=O)cccc1C(O)C(=O)(O) | 0.198E-09 | 155.3 |
| **VOPhOUA** | 225. | 9 | 7 | 6 | 1 | c1(OH)c(NO2)cHcHcHc1Cd(OH)=CdHCO(OH) | c1(O)c(N(=O)=O)cccc1C(O)=CC(=O)(O) | 0.167E-10 | 167.1 |
| **VOPhUA** | 209. | 9 | 7 | 5 | 1 | c1(OH)c(NO2)cHcHcHc1CdH=CdHCO(OH) | c1(O)c(N(=O)=O)cccc1C=CC(=O)(O) | 0.313E-08 | 140.8 |

## Table S2: radical species list

| Name | MW (g mol$^{-1}$) | Chem code (GECKO-A) |
|---|---|---|
| 1DC | 59. | CHOCH2(O.) |
| 1Na | 143. | c12cHcHcHcHc1cHcHcHc2(O.) |
| 1NaEpox | 177. | c12cHcHcHcHc1C3H-O-C3HCH(OH)C2H(O.) |
| 1NaKON | 238. | c12cHcHcHcHc1CH(ONO2)CH(O.)CH(OH)C2O |
| 1NaO | 159. | c12cHcHcHcHc1cHcHc(O.)c2(OH) |
| 1NaOBp | 193. | c12cHcHcHcHc1CH(O.)C3HCH(OH)C2H-O--O3- |
| 1NaOEpox | 193. | c12cHcHcHcHc1C3H-O-C3HCH(OH)C2(OH)(O.) |
| 1NaOKK | 191. | c12cHcHcHcHc1CH(OH)CH(O.)COC2O |
| 1NaOOBp | 209. | c12cHcHcHcHc1CH(O.)C3HCH(OH)C2(OH)-O--O3- |
| 1NaOOK | 193. | c12cHcHcHcHc1COCH(OH)CH(O.)C2H(OH) |
| 1NaOOK2 | 193. | c12cHcHcHcHc1CH(OH)CH(O.)CH(OH)C2O |
| 1NaOOOBp | 225. | c12cHcHcHcHc1C(OH)(O.)C3HCH(OH)C2(OH)-O--O3- |
| 1NaOOort | 177. | c12cHcHcHcHc1CH(OH)CH(O.)CdH=Cd2(OH) |
| 1NaOort | 161. | c12cHcHcHcHc1CdH=CdHCH(O.)C2H(OH) |
| 1NaOpar | 161. | c12cHcHcHcHc1CH(O.)CdH=CdHC2H(OH) |
| 1ONaEpox | 193. | c12cHcHcHc(OH)c1C3H-O-C3HCH(OH)C2H(O.) |
| 1ONaOBp | 209. | c12cHcHcHc(OH)c1CH(O.)C3HCH(OH)C2H-O--O3- |
| 1ONaOOK | 209. | c12cHcHcHc(OH)c1COCH(OH)CH(O.)C2H(OH) |
| 1ONaOort | 177. | c12cHcHcHc(OH)c1CdH=CdHCH(O.)C2H(OH) |
| 1ONaOpar | 177. | c12cHcHcHc(OH)c1CH(O.)CdH=CdHC2H(OH) |
| 1OPhDEnol | 193. | CHOc1cHcHcHc(OH)c1CH(O.)CdH=CdH(OH) |
| 1OPhDOD | 209. | CHOc1cHcHcHc(OH)c1CH(O.)CH(OH)CHO |
| 1OPhDUA | 207. | CO(OH)c1cHcHcHc(OH)c1CdH=CdHCO(O.) |
| 1OPhDUD | 191. | CO(O.)c1cHcHcHc(OH)c1CdH=CdHCHO |
| 1OPhUA | 179. | c1(O.)cHcHcHc(OH)c1CdH=CdHCO(OH) |
| 1OPhUD | 163. | c1HcHcHcHc(OH)c1CdH=CdHCO(O.) |
| 1OPhUEst | 191. | c12cHcHcHc(OH)c1CdH=CdHCH(O.)-O-C2O |
| 1Ph | 93. | c1HcHcHcHcHc1(O.) |
| 1PhA | 137. | CO(OH)c1cHcHcHcHc1(O.) |
| 1PhAEnol | 193. | CO(OH)c1cHcHcHcHc1CH(O.)CdH=CdH(OH) |
| 1PhAO | 181. | CO(OH)c1cHcHcHcHc1CH(OH)CH2(O.) |
| 1PhAOCD | 209. | CO(OH)c1cHcHcHcHc1CH(OH)CH2CO(O.) |
| 1PhAOOD | 225. | CO(OH)c1cHcHcHcHc1C(OH)(O.)CH(OH)CHO |
| 1PhD | 121. | CHOc1cHcHcHcHc1(O.) |
| 1PhDA | 165. | CO(OH)c1cHcHcHcHc1CO(O.) |
| 1PhDD | 149. | CHOc1cHcHcHcHc1CO(O.) |
| 1PhDEnol | 177. | CHOc1cHcHcHcHc1CH(O.)CdH=CdH(OH) |
| 1PhDKD | 191. | CHOc1cHcHcHcHc1COCH(O.)CHO |
| 1PhDKOA | 223. | CO(OH)c1cHcHcHcHc1COCH(OH)CO(O.) |
| 1PhDKOD | 207. | CO(O.)c1cHcHcHcHc1COCH(OH)CHO |
| 1PhDOCD | 193. | CO(O.)c1cHcHcHcHc1CH(OH)CH2CHO |
| 1PhDOD | 193. | CHOc1cHcHcHcHc1CH(O.)CH(OH)CHO |
| 1PhDOKA | 223. | CO(OH)CH(OH)c1cHcHcHcHc1COCO(O.) |
| 1PhDOKD | 207. | CHOCOc1cHcHcHcHc1CH(OH)CO(O.) |
| 1PhDOOD | 209. | CHOc1cHcHcHcHc1C(OH)(O.)CH(OH)CHO |
| 1PhDOOD1 | 209. | CHOc1cHcHcHcHc1C(OH)(OH)CH(O.)CHO |
| 1PhDOUA | 207. | CO(OH)c1cHcHcHcHc1Cd(OH)=CdHCO(O.) |
| 1PhDOUD | 191. | CO(O.)c1cHcHcHcHc1Cd(OH)=CdHCHO |
| 1PhDUA1 | 191. | CO(OH)c1cHcHcHcHc1CdH=CdHCO(O.) |
| 1PhDUA2 | 191. | CO(O.)c1cHcHcHcHc1CdH=CdHCO(OH) |
| 1PhDUD1 | 175. | CO(O.)c1cHcHcHcHc1CdH=CdHCHO |
| 1PhDUD2 | 175. | CHOc1cHcHcHcHc1CdH=CdHCO(O.) |
| 1PhEst | 149. | c12cHcHcHcHc1CO-O-C2H(O.) |
| 1PhKA | 165. | c1(O.)cHcHcHcHc1COCO(OH) |
| 1PhKD | 149. | c1HcHcHcHcHc1COCO(O.) |
| 1PhKKA | 193. | c1(O.)cHcHcHcHc1COCOCO(OH) |
| 1PhKOA | 195. | c1(O.)cHcHcHcHc1COCH(OH)CO(OH) |
| 1PhKOD | 179. | c1HcHcHcHcHc1COCH(OH)CO(O.) |
| 1PhKOEst | 207. | c12cHcHcHcHc1COCH(OH)CH(O.)-O-C2O |
| 1PhO | 137. | c1HcHcHcHcHc1CH(OH)CH2(O.) |
| 1PhOA | 167. | c1(O.)cHcHcHcHc1CH(OH)CO(OH) |
| 1PhOCD | 165. | c1HcHcHcHcHc1CH(OH)CH2CO(O.) |
| 1PhOCEst | 193. | c12cHcHcHcHc1CH(OH)CH2CH(O.)-O-C2O |
| 1PhOD | 151. | c1HcHcHcHcHc1CH(OH)CO(O.) |
| 1PhOKEst | 207. | c12cHcHcHcHc1COCH(O.)-O-COC2H(OH) |
| 1PhOUA | 179. | c1(O.)cHcHcHcHc1Cd(OH)=CdHCO(OH) |
| 1PhOUD | 163. | c1HcHcHcHcHc1Cd(OH)=CdHCO(O.) |
| 1PhOUEst | 191. | c12cHcHcHcHc1Cd(OH)=CdHCH(O.)-O-C2O |
| 1PhUA | 163. | c1(O.)cHcHcHcHc1CdH=CdHCO(OH) |
| 1PhUD | 147. | c1HcHcHcHcHc1CdH=CdHCO(O.) |
| 1PhUEst1 | 175. | c12cHcHcHcHc1CdH=CdHCH(O.)-O-C2O |
| 1PhUEst2 | 175. | c12cHcHcHcHc1CdH=CdHCO-O-C2H(O.) |
| 2DC | 75. | CHOCH2(OO.) |
| 2Na | 159. | c12cHcHcHcHc1cHcHcHc2(OO.) |
| 2NaKON | 254. | c12cHcHcHcHc1CH(ONO2)CH(OO.)CH(OH)C2O |
| 2NaO | 175. | c12cHcHcHcHc1cHcHc(OO.)c2(OH) |
| 2NaOBp | 209. | c12cHcHcHcHc1CH(OO.)C3HCH(OH)C2H-O--O3- |

| Name | MW (g mol$^{-1}$) | Chem code (GECKO-A) |
|---|---|---|
| 2NaOKK | 207. | c12cHcHcHcHc1CH(OH)CH(OO.)COC2O |
| 2NaOO | 193. | c12cHcHcHcHc1CH(OH)CH(OO.)CdH=Cd2(OH) ***-interm_par/ort-*** |
| 2NaOOBp | 225. | c12cHcHcHcHc1CH(OO.)C3HCH(OH)C2(OH)-O--O3- |
| 2NaOOK | 209. | c12cHcHcHcHc1COCH(OH)CH(OO.)C2H(OH) |
| 2NaOOK2 | 209. | c12cHcHcHcHc1CH(OH)CH(OO.)CH(OH)C2O |
| 2NaOOO | 209. | c12cHcHcHcHc1Cd(OH)=CdHCH(OH)C2(OH)(OO.) |
| 2NaOOOBp | 241. | c12cHcHcHcHc1C(OH)(OO.)C3HCH(OH)C2(OH)-O--O3- |
| 2NaOOort | 193. | c12cHcHcHcHc1CH(OH)CH(OO.)CdH=Cd2(OH) |
| 2NaOort | 177. | c12cHcHcHcHc1CdH=CdHCH(OO.)C2H(OH) |
| 2NaOpar | 177. | c12cHcHcHcHc1CH(OO.)CdH=CdHC2H(OH) |
| 2ONaO | 193. | c12cHcHcHc(OH)c1CdH=CdHCH(OO.)C2H(OH) ***-interm_par/ort-*** |
| 2ONaOBp | 225. | c12cHcHcHc(OH)c1CH(OO.)C3HCH(OH)C2H-O--O3- |
| 2ONaOOK | 225. | c12cHcHcHc(OH)c1COCH(OH)CH(OO.)C2H(OH) |
| 2ONaOort | 193. | c12cHcHcHc(OH)c1CdH=CdHCH(OO.)C2H(OH) |
| 2ONaOpar | 193. | c12cHcHcHc(OH)c1CH(OO.)CdH=CdHC2H(OH) |
| 2OPhDOD | 225. | CHOc1cHcHcHc(OH)c1CH(OO.)CH(OH)CHO |
| 2OPhUA | 195. | c1(OO.)cHcHcHc(OH)c1CdH=CdHCO(OH) |
| 2OPhUEst | 207. | c12cHcHcHc(OH)c1CdH=CdHCH(OO.)-O-C2O |
| 2Ph | 109. | c1HcHcHcHcHc1(OO.) |
| 2PhA | 153. | CO(OH)c1cHcHcHcHc1(OO.) |
| 2PhAO | 197. | CO(OH)c1cHcHcHcHc1CH(OH)CH2(OO.) |
| 2PhD | 137. | CHOc1cHcHcHcHc1(OO.) |
| 2PhDKD | 207. | CHOc1cHcHcHcHc1COCH(OO.)CHO |
| 2PhDOD | 209. | CHOc1cHcHcHcHc1CH(OO.)CH(OH)CHO |
| 2PhDOOD | 225. | CHOc1cHcHcHcHc1C(OH)(OH)CH(OO.)CHO |
| 2PhEst | 165. | c12cHcHcHcHc1CO-O-C2H(OO.) |
| 2PhKA | 181. | c1(OO.)cHcHcHcHc1COCO(OH) |
| 2PhKKA | 209. | c1(OO.)cHcHcHcHc1COCOCO(OH) |
| 2PhKOA | 211. | c1(OO.)cHcHcHcHc1COCH(OH)CO(OH) |
| 2PhKOEst | 223. | c12cHcHcHcHc1COCH(OH)CH(OO.)-O-C2O |
| 2PhO | 153. | c1HcHcHcHcHc1CH(OH)CH2(OO.) |
| 2PhOA | 183. | c1(OO.)cHcHcHcHc1CH(OH)CO(OH) |
| 2PhOCEst | 209. | c12cHcHcHcHc1CH(OH)CH2CH(OO.)-O-C2O |
| 2PhOKEst | 223. | c12cHcHcHcHc1COCH(OO.)-O-COC2H(OH) |
| 2PhOUA | 195. | c1(OO.)cHcHcHcHc1Cd(OH)=CdHCO(OH) |
| 2PhOUEst | 207. | c12cHcHcHcHc1Cd(OH)=CdHCH(OO.)-O-C2O |
| 2PhUA | 179. | c1(OO.)cHcHcHcHc1CdH=CdHCO(OH) |
| 2PhUEst1 | 191. | c12cHcHcHcHc1CdH=CdHCH(OO.)-O-C2O |
| 2PhUEst2 | 191. | c12cHcHcHcHc1CdH=CdHCO-O-C2H(OO.) |
| 3GLY | 89. | CHOCO(OO.) |
| 3OPhU | 179. | c1HcHcHcHc(OH)c1CdH=CdHCO(OO.) |
| 3OPhUA | 223. | CO(OH)c1cHcHcHc(OH)c1CdH=CdHCO(OO.) |
| 3OPhUD | 207. | CO(OO.)c1cHcHcHc(OH)c1CdH=CdHCHO |
| 3PhA | 181. | CO(OH)c1cHcHcHcHc1CO(OO.) |
| 3PhAOC | 225. | CO(OH)c1cHcHcHcHc1CH(OH)CH2CO(OO.) |
| 3PhD | 165. | CHOc1cHcHcHcHc1CO(OO.) |
| 3PhK | 165. | c1HcHcHcHcHc1COCO(OO.) |
| 3PhKO | 195. | c1HcHcHcHcHc1COCH(OH)CO(OO.) |
| 3PhKOA | 239. | CO(OH)c1cHcHcHcHc1COCH(OH)CO(OO.) |
| 3PhKOD | 223. | CO(OO.)c1cHcHcHcHc1COCH(OH)CHO |
| 3PhN | 212. | c1HcHcHcHcHc1CH(ONO2)CO(OO.) |
| 3PhND | 240. | CO(OO.)c1cHcHcHcHc1CH(ONO2)CHO |
| 3PhO | 167. | c1HcHcHcHcHc1CH(OH)CO(OO.) |
| 3PhOC | 181. | c1HcHcHcHcHc1CH(OH)CH2CO(OO.) |
| 3PhOCD | 209. | CO(OO.)c1cHcHcHcHc1CH(OH)CH2CHO |
| 3PhOKA | 239. | CO(OH)CH(OH)c1cHcHcHcHc1COCO(OO.) |
| 3PhOKD | 223. | CHOCOc1cHcHcHcHc1CH(OH)CO(OO.) |
| 3PhOU | 179. | c1HcHcHcHcHc1Cd(OH)=CdHCO(OO.) |
| 3PhOUA | 223. | CO(OH)c1cHcHcHcHc1Cd(OH)=CdHCO(OO.) |
| 3PhOUD | 207. | CO(OO.)c1cHcHcHcHc1Cd(OH)=CdHCHO |
| 3PhU | 163. | c1HcHcHcHcHc1CdH=CdHCO(OO.) |
| 3PhUA1 | 207. | CO(OH)c1cHcHcHcHc1CdH=CdHCO(OO.) |
| 3PhUA2 | 207. | CO(OO.)c1cHcHcHcHc1CdH=CdHCO(OH) |
| 3PhUD1 | 191. | CO(OO.)c1cHcHcHcHc1CdH=CdHCHO |
| 3PhUD2 | 191. | CHOc1cHcHcHcHc1CdH=CdHCO(OO.) |
| 4NaO | 145. | c12cHcHcHcHc1CdH=CdHC.HC2H(OH) |
| 4NaOBp | 177. | c12cHcHcHcHc1CH.C3HCH(OH)C2H-O--O3- |
| 4NaOOBp | 193. | c12cHcHcHcHc1CH.C3HCH(OH)C2(OH)-O--O3- |
| 4NaOPEN1 | 159. | C.Oc1cHcHcHcHc1CdH=CdHCHO |
| 4NaOPEN2 | 159. | CHOc1cHcHcHcHc1CdH=CdHC.O |
| 4NaOPENO | 177. | C.Oc1cHcHcHcHc1CH(OH)CH2CHO |
| 4NaOPENOL | 175. | C.Oc1cHcHcHcHc1Cd(OH)=CdHCHO |
| 4ONaOBp | 193. | c12cHcHcHc(OH)c1CH.C3HCH(OH)C2H-O--O3- |
| 4ONaOPEN | 175. | C.Oc1cHcHcHc(OH)c1CdH=CdHCHO |
| 4PhDKOD | 191. | C.Oc1cHcHcHcHc1COCH(OH)CHO |
| 4PhODKD | 191. | C.OCOc1cHcHcHcHc1CH(OH)CHO |
| 5OPhDCrg | 180. | CHOc1cHcHcHc(OH)c1CH2C.H(OO.) |
| 5PhDCrg | 164. | CHOc1cHcHcHcHc1CH2C.H(OO.) |

## Table S3: Detailed naphthalene chemical scheme

| reaction ID | reaction | | | kinetic type | kinetic values |
|---|---|---|---|---|---|
| **BLOCK 1: NAPH AND NaV CHEMISTRY** | | | | | |
| B1-001 | NAPH + HO | → | 4NaO | *ARR2* | 1.105E-12 -908.0 |
| B1-002 | 4NaO + NO2 | → | NaV | *ARR1* | 3.6E-11 |
| B1-003 | NaV | → | 1Na + NO | *PHOTO* | 4.536E-04 |
| B1-004 | NaV + HO | → | 0.22 NaVO + 0.22 HO2 | *ARR1* | 4.45E-12 |
| B1-005 | 4NaO | → | 0.255 NaO + 0.255 HO2 + 0.079 4NaOBp + 0.546 2NaOort + 0.120 2NaOpar | *ARR1(O2)* | 4.47E-16 |
| B1-006 | 1Na + O3 | → | 2Na | *ARR1* | 2.86E-13 |
| B1-007 | 1Na + NO2 | → | NaVO | *ARR1* | 2.08E-12 |
| B1-008 | 1Na + HO2 | → | NaO | *ARR1* | 2.30E-13 |
| B1-009 | 2Na + NO | → | 1Na + NO2 | *ARR2* | 2.7E-12 -360.0 |
| B1-010 | 2Na + NO2 | → | 1Na + NO3 | *ARR3* | 6.143E-09 -1.1 0.00 |
| B1-011 | 2Na + NO3 | → | 1Na + NO2 | *ARR2* | 8.90E-12 390.0 |
| B1-012 | 2Na + HO2 | → | NaH | *ARR2* | 2.096E-13 -1300.0 |
| B1-013 | 2Na + MO2 | → | 0.80 1Na + 0.20 NaO + CH2O + 0.80 HO2 | *ARR2* | 1.03E-13 -324.0 |
| ***BLOCK 2: 2NaOpar CHEMISTRY (PARA RO2)*** | | | | | |
| B2-001 | 2NaOpar + NO | → | 0.82 1NaOpar + 0.18 NaONpar + 0.82 NO2 | *ARR2* | 2.7E-12 -360.0 |
| B2-002 | 2NaOpar + HO2 | → | NaOHpar | *ARR2* | 2.577E-13 -1300.0 |
| B2-003 | 2NaOpar + NO3 | → | 1NaOpar + NO2 | *ARR2* | 8.90E-12 390.0 |
| B2-004 | 2NaOpar + MO2 | → | 0.60 1NaOpar + 0.20 NaOOpar + 0.20 NaOKpar + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.00E-13 -663.59 |
| B2-005 | 1NaOpar | → | NaOKpar + HO2 | *ARR1(O2)* | 2.50E-14 300.0 |
| B2-006 | NaOKpar + HO | → | 0.225 NaQuin + 0.775 2NaOOK + 0.225 HO2 | *ARR1* | 8.80E-11 |
| B2-007 | 2NaOOK + NO | → | 0.875 1NaOOK + 0.125 NaNOOK + 0.875 NO2 | *ARR2* | 2.7E-12 -360.0 |
| B2-008 | 2NaOOK + HO2 | → | NaHOOK | *ARR2* | 2.659E-13 -1300.0 |
| B2-009 | 2NaOOK + NO3 | → | 1NaOOK + NO2 | *ARR2* | 8.90E-12 390.0 |
| B2-010 | 2NaOOK + MO2 | → | 0.60 1NaOOK + 0.20 NaOOOK + 0.20 NaOOKK + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -791.0 |
| B2-011 | 1NaOOK | → | 0.57 PhODKD + 0.43 PhDKOD + HO2 | *ARR3* | 1.12E+09 1.7 2301.0 |
| B2-012 | PhODKD + HO | → | 0.82 4PhODKD + 0.18 PhKDKD + 0.18 HO2 | *ARR1* | 3.56E-11 |
| B2-013 | PhODKD + NO3 | → | PhKDKD + HNO3 + HO2 | *ARR1* | 2.87E-13 |
| B2-014 | 4PhODKD | → | 0.40 2PhOKEst + 0.60 3PhOKD | *ARR1* | 1.00E+06 |
| B2-015 | 2PhOKEst + NO | → | 1PhOKEst + NO2 | *ARR2* | 2.7E-12 -360.0 |
| B2-016 | 2PhOKEst + HO2 | → | 0.540 PhOKHEst + 0.460 PhOKAnhy + 0.20 HO + 0.20 HO2 | *ARR2* | 2.62E-13 -1300.0 |
| B2-017 | 2PhOKEst + NO3 | → | 1PhOKEst + NO2 | *ARR2* | 8.90E-12 390.0 |
| B2-018 | 2PhOKEst + MO2 | → | 0.60 1PhOKEst + 0.20 PhOKAnhy + 0.20 PhOKOEst + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -955.0 |
| B2-019 | 1PhOKEst | → | 3PhOKA | *ARR3* | 8.00E+10 1.7 3723.0 |
| B2-020 | 3PhOKA + NO | → | 1PhDOKA + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B2-021 | 3PhOKA + NO2 | → | PhPOKA | *ARR3* | 6.143E-09 -1.1 0.0 |
| B2-022 | 3PhOKA + NO3 | → | 1PhDOKA + NO2 | *ARR2* | 8.90E-12 305.0 |
| B2-023 | 3PhOKA + HO2 | → | 0.65 PhGOKA + 0.15 PhAOKA + 0.20 1PhDOKA + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 -730.0 |
| B2-024 | 3PhOKA + MO2 | → | 0.80 1PhDOKA + 0.20 PhAOKA + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B2-025 | 3PhOKD + NO | → | 1PhDOKD + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B2-026 | 3PhOKD + NO2 | → | PhPOKD | *ARR3* | 6.143E-09 -1.1 0.0 |
| B2-027 | 3PhOKD + NO3 | → | 1PhDOKD + NO2 | *ARR2* | 8.90E-12 305.0 |
| B2-028 | 3PhOKD + HO2 | → | 0.65 PhGOKD + 0.15 PhAOKD + 0.20 1PhDOKD + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 -730.0 |
| B2-029 | 3PhOKD + MO2 | → | 0.80 1PhDOKD + 0.20 PhAOKD + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| B2-030 | 1PhDOKA | → | 0.60 PhOKAnhy + 0.60 HO + 0.20 2PhOA + 0.2 CO + 0.2 CO2 + 0.20 PhDKA + 0.2 CO2 + 0.2 HO2 | *ARR1* | 1.00E+06 | | |
| B2-031 | 1PhDOKD | → | 0.60 PhOKAnhy + 0.60 HO2 + 0.20 PhKDD + 0.20 CO2 + 0.20 HO2 + 0.20 3PhO + 0.20 CO2 + 0.20 CO | *ARR1* | 1.00E+06 | | |
| B2-032 | 2PhOA + NO | → | 1PhOA + NO2 | *ARR2* | 2.7E-12 | -360.0 | |
| B2-033 | 2PhOA + NO2 | → | 1PhOA + NO3 | *ARR3* | 6.143E-09 | -1.1 | 0.0 |
| B2-034 | 2PhOA + NO3 | → | 1PhOA + NO2 | *ARR2* | 8.90E-12 | 390.0 | |
| B2-035 | 2PhOA + HO2 | → | HPhOA | *ARR2* | 2.335E-13 | -1300.0 | |
| B2-036 | 2PhOA + MO2 | → | 0.80 1PhOA + 0.20 OPhOA + CH2O + 0.80 HO2 | *ARR2* | 1.03E-13 | -398.0 | |
| B2-037 | 1PhOA + O3 | → | 2PhOA | *ARR1* | 2.86E-13 | | |
| B2-038 | 1PhOA + NO2 | → | VOPhOA | *ARR1* | 2.08E-12 | | |
| B2-039 | 1PhOA + HO2 | → | OPhOA | *ARR1* | 2.30E-13 | | |
| B2-040 | 3PhO + NO | → | 1PhOD + NO2 | *ARR2* | 7.50E-12 | -290.0 | |
| B2-041 | 3PhO + NO2 | → | PhOP | *ARR3* | 6.143E-09 | -1.1 | 0.0 |
| B2-042 | 3PhO + NO3 | → | 1PhOD + NO2 | *ARR2* | 8.90E-12 | 305.0 | |
| B2-043 | 3PhO + HO2 | → | 0.65 PhOG + 0.15 PhOA + 0.20 1PhOD + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 | -730.0 | |
| B2-044 | 3PhO + MO2 | → | 0.80 1PhOD + 0.20 PhOA + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 | -508.0 | |
| B2-045 | 1PhOD | → | PhD + CO2 + HO2 | *ARR1* | 1.00E+06 | | |
| B2-046 | PhOKAnhy | → | PhAOKA | *ARR1(H2O)* | 2.50E-22 | | |
| B2-047 | PhKDKD + HO | → | 0.6 PhKKAnhy + 0.24 HO + 0.36 HO2 + 0.2 2PhKA + 0.20 CO + 0.20 CO2 + 0.2 3PhK + 0.20 CO + 0.20 CO2 | *ARR1* | 2.59E-11 | | |
| B2-048 | 2PhKA + NO | → | 1PhKA + NO2 | *ARR2* | 2.7E-12 | -360.0 | |
| B2-049 | 2PhKA + NO2 | → | 1PhKA + NO3 | *ARR3* | 6.143E-09 | -1.1 | 0.0 |
| B2-050 | 2PhKA + NO3 | → | 1PhKA + NO2 | *ARR2* | 8.90E-12 | 390.0 | |
| B2-051 | 2PhKA + HO2 | → | HPhKA | *ARR2* | 2.335E-13 | -1300.0 | |
| B2-052 | 2PhKA + MO2 | → | 0.80 1PhKA + 0.20 OPhKA + CH2O + 0.80 HO2 | *ARR2* | 1.03E-13 | -398.0 | |
| B2-053 | 1PhKA + O3 | → | 2PhKA | *ARR1* | 2.86E-13 | | |
| B2-054 | 1PhKA + NO2 | → | VOPhKA | *ARR1* | 2.08E-12 | | |
| B2-055 | 1PhKA + HO2 | → | OPhKA | *ARR1* | 2.30E-13 | | |
| B2-056 | 3PhK + NO | → | 1PhKD + NO2 | *ARR2* | 7.50E-12 | -290.0 | |
| B2-057 | 3PhK + NO2 | → | PhKP | *ARR3* | 6.143E-09 | -1.1 | 0.0 |
| B2-058 | 3PhK + NO3 | → | 1PhKD + NO2 | *ARR2* | 8.90E-12 | 305.0 | |
| B2-059 | 3PhK + HO2 | → | 0.65 PhKG + 0.15 PhKA + 0.20 1PhKD + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 | -730.0 | |
| B2-060 | 3PhK + MO2 | → | 0.80 1PhKD + 0.20 PhKA + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 | -508.0 | |
| B2-061 | 1PhKD | → | 2Ph + CO2 + CO | *ARR1* | 1.00E+06 | | |
| B2-062 | 2Ph + NO | → | 1Ph + NO2 | *ARR2* | 2.7E-12 | -360.0 | |
| B2-063 | 2Ph + NO2 | → | 1Ph + NO3 | *ARR3* | 6.143E-09 | -1.1 | 0.0 |
| B2-064 | 2Ph + NO3 | → | 1Ph + NO2 | *ARR2* | 8.90E-12 | 390.0 | |
| B2-065 | 2Ph + HO2 | → | HPh | *ARR2* | 2.335E-13 | -1300.0 | |
| B2-066 | 2Ph + MO2 | → | 0.80 1Ph + 0.20 OPh + CH2O + 0.80 HO2 | *ARR2* | 1.03E-13 | -398.0 | |
| B2-067 | 1Ph + O3 | → | 2Ph | *ARR1* | 2.86E-13 | | |
| B2-068 | 1Ph + NO2 | → | VOPh | *ARR1* | 2.08E-12 | | |
| B2-069 | 1Ph + HO2 | → | OPh | *ARR1* | 2.30E-13 | | |
| B2-070 | PhKKAnhy | → | PhKAKA | *ARR1(H2O)* | 2.50E-22 | | |
| B2-071 | PhDKOD + HO | → | 0.82 4PhDKOD + 0.18 PhDKKD + 0.18 HO2 | *ARR1* | 3.04E-11 | | |
| B2-072 | PhDKOD + NO3 | → | PhDKKD + HNO3 + HO2 | *ARR1* | 1.92E-13 | | |
| B2-073 | 4PhDKOD | → | 0.40 2PhKOEst + 0.60 3PhKOD | *ARR1* | 1.00E+06 | | |
| B2-074 | 2PhKOEst + NO | → | 1PhKOEst + NO2 | *ARR2* | 2.7E-12 | -360.0 | |
| B2-075 | 2PhKOEst + HO2 | → | 0.540 PhKOHEst + 0.460 PhKOAnhy + 0.20 HO + 0.20 HO2 | *ARR2* | 2.62E-13 | -1300.0 | |
| B2-076 | 2PhKOEst + NO3 | → | 1PhKOEst + NO2 | *ARR2* | 8.90E-12 | 390.0 | |
| B2-077 | 2PhKOEst + MO2 | → | 0.60 1PhKOEst + 0.20 PhKOAnhy + 0.20 PhKOOEst + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 | -955.0 | |
| B2-078 | 1PhKOEst | → | 3PhKOA | *ARR3* | 8.00E+10 | 1.7 | 3723.0 |
| B2-079 | 3PhKOA + NO | → | 1PhDKOA + NO2 | *ARR2* | 7.50E-12 | -290.0 | |

| | | | | | |
|---|---|---|---|---|---|
| B2-080 | 3PhKOA + NO2 | → | PhPKOA | *ARR3* | 6.143E-09 -1.1 0.0 |
| B2-081 | 3PhKOA + NO3 | → | 1PhDKOA + NO2 | *ARR2* | 8.90E-12 305.0 |
| B2-082 | 3PhKOA + HO2 | → | 0.65 PhGKOA + 0.15 PhAKOA + 0.20 1PhDKOA + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 -730.0 |
| B2-083 | 3PhKOA + MO2 | → | 0.80 1PhDKOA + 0.20 PhAKOA + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B2-084 | 3PhKOD + NO | → | 1PhDKOD + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B2-085 | 3PhKOD + NO2 | → | PhPKOD | *ARR3* | 6.143E-09 -1.1 0.0 |
| B2-086 | 3PhKOD + NO3 | → | 1PhDKOD + NO2 | *ARR2* | 8.90E-12 305.0 |
| B2-087 | 3PhKOD + HO2 | → | 0.65 PhGKOD + 0.15 PhAKOD + 0.20 1PhDKOD + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 -730.0 |
| B2-088 | 3PhKOD + MO2 | → | 0.80 1PhDKOD + 0.20 PhAKOD + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B2-089 | 1PhDKOA | → | 0.60 PhKOAnhy + 0.60 HO + 0.20 PhAKD + 0.2 CO2 + 0.2 HO2 + 0.20 2PhKOA + 0.2 CO2 | *ARR1* | 1.00E+06 |
| B2-090 | 1PhDKOD | → | 0.60 PhKOAnhy + 0.60 HO2 + 0.20 3PhKO + 0.20 CO2 + 0.20 PhKDD + 0.20 CO2 + 0.20 HO2 | *ARR1* | 1.00E+06 |
| B2-091 | 2PhKOA + NO | → | 1PhKOA + NO2 | *ARR2* | 2.7E-12 -360.0 |
| B2-092 | 2PhKOA + NO2 | → | 1PhKOA + NO3 | *ARR3* | 6.143E-09 -1.1 0.0 |
| B2-093 | 2PhKOA + NO3 | → | 1PhKOA + NO2 | *ARR2* | 8.90E-12 390.0 |
| B2-094 | 2PhKOA + HO2 | → | HPhKOA | *ARR2* | 2.335E-13 -1300.0 |
| B2-095 | 2PhKOA + MO2 | → | 0.80 1PhKOA + 0.20 OPhKOA + CH2O + 0.80 HO2 | *ARR2* | 1.03E-13 -398.0 |
| B2-096 | 1PhKOA + O3 | → | 2PhKOA | *ARR1* | 2.86E-13 |
| B2-097 | 1PhKOA + NO2 | → | VOPhKOA | *ARR1* | 2.08E-12 |
| B2-098 | 1PhKOA + HO2 | → | OPhKOA | *ARR1* | 2.30E-13 |
| B2-099 | 3PhKO + NO | → | 1PhKOD + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B2-100 | 3PhKO + NO2 | → | PhKOP | *ARR3* | 6.143E-09 -1.1 0.0 |
| B2-101 | 3PhKO + NO3 | → | 1PhKOD + NO2 | *ARR2* | 8.90E-12 305.0 |
| B2-102 | 3PhKO + HO2 | → | 0.65 PhKOG + 0.15 PhKOA + 0.20 1PhKOD + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 -730.0 |
| B2-103 | 3PhKO + MO2 | → | 0.80 1PhKOD + 0.20 PhKOA + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B2-104 | 1PhKOD | → | PhKD + CO2 + HO2 | *ARR1* | 1.00E+06 |
| B2-105 | PhKOAnhy | → | PhAKOA | *ARR1(H2O)* | 2.50E-22 |
| B2-106 | PhDKKD + HO | → | 0.60 PhKKAnhy + 0.24 HO + 0.36 HO2 + 0.12 2Ph + 0.24 CO + 0.24 CO2 + 0.12 2PhD + 0.24 CO + 0.12 CO2 + 0.08 2PhA + 0.16 CO + 0.08 CO2 + 0.08 2PhKKA + 0.08 CO2 | *ARR1* | 2.51E-11 |
| B2-107 | 2PhKKA + NO | → | 1PhKKA + NO2 | *ARR2* | 2.7E-12 -360.0 |
| B2-108 | 2PhKKA + NO2 | → | 1PhKKA + NO3 | *ARR3* | 6.143E-09 -1.1 0.0 |
| B2-109 | 2PhKKA + NO3 | → | 1PhKKA + NO2 | *ARR2* | 8.90E-12 390.0 |
| B2-110 | 2PhKKA + HO2 | → | HPhKKA | *ARR2* | 2.335E-13 -1300.0 |
| B2-111 | 2PhKKA + MO2 | → | 0.80 1PhKKA + 0.20 OPhKKA + CH2O + 0.80 HO2 | *ARR2* | 1.03E-13 -398.0 |
| B2-112 | 1PhKKA + O3 | → | 2PhKKA | *ARR1* | 2.86E-13 |
| B2-113 | 1PhKKA + NO2 | → | VOPhKKA | *ARR1* | 2.08E-12 |
| B2-114 | 1PhKKA + HO2 | → | OPhKKA | *ARR1* | 2.30E-13 |
| B2-115 | PhKDD + HO | → | 0.60 PhKAnhy + 0.24 HO + 0.36 HO2 + 0.12 2Ph + 0.12 CO + 0.24 CO2 + 0.12 2PhD + 0.12 CO + 0.12 CO2 + 0.08 2PhA + 0.08 CO + 0.08 CO2 + 0.08 2PhKA + 0.08 CO2 | *ARR1* | 2.51E-11 |

***BLOCK 3: 2NaOort (ORTHO RO2) AND NaOPEN CHEMISTRY***

| | | | | | |
|---|---|---|---|---|---|
| B3-001 | 2NaOort + NO | → | 0.875 1NaOort + 0.125 NaONort + 0.875 NO2 | *ARR2* | 2.7E-12 -360.0 |
| B3-002 | 2NaOort + HO2 | → | NaOHort | *ARR2* | 2.659E-13 -1300.0 |
| B3-003 | 2NaOort + NO3 | → | 1NaOort + NO2 | *ARR2* | 8.90E-12 390.0 |
| B3-004 | 2NaOort + MO2 | → | 0.60 1NaOort + 0.20 NaOOort + 0.20 NaOKort + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -791.0 |
| B3-005 | 2NaOort | → | NaOPEN + HO | *ARR2* | 1.90E11 9750.0 |
| B3-006 | 1NaOort | → | NaOPEN + HO2 | *ARR3* | 1.12E+09 1.7 2301.0 |

| | | | | | |
|---|---|---|---|---|---|
| B3-007 | NaOPEN + HO | → | 0.52 2PhDOD + 0.28 4NaOPEN1 + 0.20 4NaOPEN2 | *ARR1* | 6.50E-11 |
| B3-008 | NaOPEN | → | 3PhU + CO + HO2 | *PHOTO* | 2.2690E-05 |
| B3-009 | NaOPEN | → | PhDD + 2.0 CO + 2.0 HO2 | *PHOTO* | 6.4685E-06 |
| B3-010 | NaOPEN | → | 5PhDCrg + CO | *PHOTO* | 6.2783E-06 |
| B3-011 | NaOPEN | → | 4NaOPEN2 + HO2 | *PHOTO* | 6.2783E-06 |
| B3-012 | 5PhDCrg | → | 0.625 PhDCA + 0.375 PhDCD + 0.375 H2O2 | *ARR1(H2O)* | 1.205E-14 |
| B3-013 | 5PhDCrg + NO | → | PhDCD + NO2 | *ARR1* | 0.600E-13 |
| B3-014 | 5PhDCrg + NO2 | → | PhDCD + NO3 | *ARR1* | 0.200E-11 |
| B3-015 | 5PhDCrg + CO | → | PhDCD + CO2 | *ARR1* | 0.219E-19 |
| B3-016 | 5PhDCrg + HNO3 | → | PhDCD + HNO4 | *ARR1* | 0.540E-09 |
| B3-017 | 5PhDCrg + O3 | → | PhDCD | *ARR1* | 0.152E-11 |
| B3-018 | 5PhDCrg | → | PhDCD + HO | *ARR1* | 0.114E+03 |
| B3-019 | 2PhDOD + NO | → | 0.810 1PhDOD + 0.190 PhDNOD + 0.810 NO2 | *ARR2* | 2.7E-12 -360.0 |
| B3-020 | 2PhDOD + NO3 | → | 1PhDOD + NO2 | *ARR2* | 8.90E-12 390.0 |
| B3-021 | 2PhDOD + HO2 | → | PhDHOD | *ARR2* | 2.66E-13 -1300.0 |
| B3-022 | 2PhDOD + MO2 | → | 0.60 1PhDOD + 0.20 PhDOOD + 0.20 PhDKOD + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -1031.0 |
| B3-023 | 2PhDOD + HO | → | 1PhDOD + HO2 | *ARR2* | 3.70E-11 -350.0 |
| B3-024 | 1PhDOD | → | GLYOX + PhDD + HO2 | *ARR3* | 1.12E+09 1.7 1644.0 |
| B3-025 | 4NaOPEN1 | → | 0.40 2PhUEst1 + 0.60 3PhUD1 | *ARR1* | 1.00E+06 |
| B3-026 | 2PhUEst1 + NO | → | 1PhUEst1 + NO2 | *ARR2* | 2.7E-12 -360.0 |
| B3-027 | 2PhUEst1 + HO2 | → | 0.540 PhUHEst1 + 0.460 PhUAnhy + 0.20 HO + 0.20 HO2 | *ARR2* | 2.62E-13 -1300.0 |
| B3-028 | 2PhUEst1 + NO3 | → | 1PhUEst1 + NO2 | *ARR2* | 8.90E-12 390.0 |
| B3-029 | 2PhUEst1 + MO2 | → | 0.60 1PhUEst1 + 0.20 PhUAnhy + 0.20 PhUOEst1 + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -955.0 |
| B3-030 | 1PhUEst1 | → | 3PhUA1 | *ARR3* | 8.00E+10 1.7 3723.0 |
| B3-031 | 3PhUA1 + NO | → | 1PhDUA1 + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B3-032 | 3PhUA1 + NO2 | → | PhPUA1 | *ARR3* | 6.143E-09 -1.1 0.0 |
| B3-033 | 3PhUA1 + NO3 | → | 1PhDUA1 + NO2 | *ARR2* | 8.90E-12 305.0 |
| B3-034 | 3PhUA1 + HO2 | → | 0.65 PhGUA1 + 0.15 PhAUA + 0.20 1PhDUA1 + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 -730.0 |
| B3-035 | 3PhUA1 + MO2 | → | 0.80 1PhDUA1 + 0.20 PhAUA + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B3-036 | 1PhDUA1 | → | 0.60 PhUAnhy + 0.60 HO + 0.40 PhAD + 0.4 CO + 0.4 CO2 + 0.4 HO2 | *ARR1* | 1.00E+06 |
| B3-037 | 3PhUD1 + NO | → | 1PhDUD1 + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B3-038 | 3PhUD1 + NO2 | → | PhPUD1 | *ARR3* | 6.143E-09 -1.1 0.0 |
| B3-039 | 3PhUD1 + NO3 | → | 1PhDUD1 + NO2 | *ARR2* | 8.90E-12 305.0 |
| B3-040 | 3PhUD1 + HO2 | → | 0.65 PhGUD1 + 0.15 PhAUD1 + 0.20 1PhDUD1 + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 -730.0 |
| B3-041 | 3PhUD1 + MO2 | → | 0.80 1PhDUD1 + 0.20 PhAUD1 + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B3-042 | 1PhDUD1 | → | 0.60 PhUAnhy + 0.60 HO2 + 0.40 3PhU + 0.40 CO2 | *ARR1* | 1.00E+06 |
| B3-043 | 3PhU + NO | → | 1PhUD + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B3-044 | 3PhU + NO2 | → | PhUP | *ARR3* | 6.143E-09 -1.1 0.0 |
| B3-045 | 3PhU + NO3 | → | 1PhUD + NO2 | *ARR2* | 8.90E-12 305.0 |
| B3-046 | 3PhU + HO2 | → | 0.65 PhUG + 0.15 PhUA + 0.20 1PhUD + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 -730.0 |
| B3-047 | 3PhU + MO2 | → | 0.80 1PhUD + 0.20 PhUA + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B3-048 | 1PhUD | → | PhD + CO + CO2 + HO2 | *ARR1* | 1.00E+06 |
| B3-049 | PhUAnhy | → | PhAUA | *ARR1(H2O)* | 2.50E-22 |
| B3-050 | 4NaOPEN2 | → | 0.40 2PhUEst2 + 0.60 3PhUD2 | *ARR1* | 1.00E+06 |
| B3-051 | 2PhUEst2 + NO | → | 1PhUEst2 + NO2 | *ARR2* | 2.7E-12 -360.0 |
| B3-052 | 2PhUEst2 + HO2 | → | 0.540 PhUHEst2 + 0.460 PhUAnhy + 0.20 HO + 0.20 HO2 | *ARR2* | 2.62E-13 -1300.0 |
| B3-053 | 2PhUEst2 + NO3 | → | 1PhUEst2 + NO2 | *ARR2* | 8.90E-12 390.0 |
| B3-054 | 2PhUEst2 + MO2 | → | 0.60 1PhUEst2 + 0.20 PhUAnhy + 0.20 PhUOEst2 + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -1010.0 |
| B3-055 | 1PhUEst2 | → | 3PhUA2 | *ARR3* | 8.00E+10 1.7 3723.0 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| B3-056 | 3PhUA2 + NO | → | 1PhDUA2 + NO2 | *ARR2* | 7.50E-12 | -290.0 | |
| B3-057 | 3PhUA2 + NO2 | → | PhPUA2 | *ARR3* | 6.143E-09 | -1.1 | 0.0 |
| B3-058 | 3PhUA2 + NO3 | → | 1PhDUA2 + NO2 | *ARR2* | 8.90E-12 | 305.0 | |
| B3-059 | 3PhUA2 + HO2 | → | 0.65 PhGUA2 + 0.15 PhAUA + 0.20 1PhDUA2 + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 | -730.0 | |
| B3-060 | 3PhUA2 + MO2 | → | 0.80 1PhDUA2 + 0.20 PhAUA + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 | -508.0 | |
| B3-061 | 1PhDUA2 | → | 0.60 PhUAnhy + 0.60 HO + 0.40 2PhUA + 0.40 CO2 | *ARR1* | 1.00E+06 | | |
| B3-062 | 2PhUA + NO | → | 1PhUA + NO2 | *ARR2* | 2.7E-12 | -360.0 | |
| B3-063 | 2PhUA + NO2 | → | 1PhUA + NO3 | *ARR3* | 6.143E-09 | -1.1 | 0.0 |
| B3-064 | 2PhUA + NO3 | → | 1PhUA + NO2 | *ARR2* | 8.90E-12 | 390.0 | |
| B3-065 | 2PhUA + HO2 | → | HPhUA | *ARR2* | 2.335E-13 | -1300.0 | |
| B3-066 | 2PhUA + MO2 | → | 0.80 1PhUA + 0.20 OPhUA + CH2O + 0.80 HO2 | *ARR2* | 1.03E-13 | -398.0 | |
| B3-067 | 1PhUA + O3 | → | 2PhUA | *ARR1* | 2.86E-13 | | |
| B3-068 | 1PhUA + NO2 | → | VOPhUA | *ARR1* | 2.08E-12 | | |
| B3-069 | 1PhUA + HO2 | → | OPhUA | *ARR1* | 2.30E-13 | | |
| B3-070 | 3PhUD2 + NO | → | 1PhDUD2 + NO2 | *ARR2* | 7.50E-12 | -290.0 | |
| B3-071 | 3PhUD2 + NO2 | → | PhPUD2 | *ARR3* | 6.143E-09 | -1.1 | 0.0 |
| B3-072 | 3PhUD2 + NO3 | → | 1PhDUD2 + NO2 | *ARR2* | 8.90E-12 | 305.0 | |
| B3-073 | 3PhUD2 + HO2 | → | 0.65 PhGUD2 + 0.15 PhAUD2 + 0.20 1PhDUD2 + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 | -730.0 | |
| B3-074 | 3PhUD2 + MO2 | → | 0.80 1PhDUD2 + 0.20 PhAUD2 + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 | -508.0 | |
| B3-075 | 1PhDUD2 | → | 0.60 PhUAnhy + HO2 + 0.40 PhDD + 0.4 CO + 0.4 CO2 | *ARR1* | 1.00E+06 | | |

***BLOCK 4: 4NaOBp CHEMISTRY (PEROXY BRIDGE)***

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| B4-001 | 4NaOBp | → | 0.75 2NaOBp + 0.25 1NaEpox | *ARR1* | 1.0E+06 | | |
| B4-002 | 2NaOBp + NO | → | 0.91 1NaOBp + 0.09 NaONBp + 0.91 NO2 | *ARR2* | 2.7E-12 | -360.0 | |
| B4-003 | 2NaOBp + HO2 | → | NaOHBp | *ARR2* | 2.447E-13 | -1300.0 | |
| B4-004 | 2NaOBp + NO3 | → | 1NaOBp + NO2 | *ARR2* | 8.90E-12 | 390.0 | |
| B4-005 | 2NaOBp + MO2 | → | 0.60 1NaOBp + 0.20 NaOOBp + 0.20 NaOKBp + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 | -598.0 | |
| B4-006 | 1NaOBp | → | 1PhDOD | *ARR3* | 1.12E+09 | 1.7 | 2413.0 |
| B4-007 | 1NaEpox | → | 1PhDEnol | *ARR3* | 1.12E+09 | 1.7 | 2301.0 |
| B4-008 | 1PhDEnol | → | 4NaOPENO | *ARR2* | 6.00E+10 | 2990.0 | |
| B4-009 | 1PhDEnol | → | PhDD + 2DC | *ARR3* | 1.12E+09 | 1.7 | 4830.9 |
| B4-010 | 4NaOPENO | → | 0.40 2PhOCEst + 0.60 3PhOCD | *ARR1* | 1.00E+06 | | |
| B4-011 | 2PhOCEst + NO | → | 1PhOCEst + NO2 | *ARR2* | 2.7E-12 | -360.0 | |
| B4-012 | 2PhOCEst + HO2 | → | 0.540 PhOCHEst + 0.460 PhOCAnhy + 0.20 HO + 0.20 HO2 | *ARR2* | 2.62E-13 | -1300.0 | |
| B4-013 | 2PhOCEst + NO3 | → | 1PhOCEst + NO2 | *ARR2* | 8.90E-12 | 390.0 | |
| B4-014 | 2PhOCEst + MO2 | → | 0.60 1PhOCEst + 0.20 PhOCAnhy + 0.20 PhOCOEst + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 | -955.0 | |
| B4-015 | 1PhOCEst | → | PhOCAnhy + HO2 | *ARR2(O2)* | 2.5E-14 | 300.0 | |
| B4-016 | 1PhOCEst | → | 3PhAOC | *ARR3* | 8.00E+10 | 1.7 | 3723.0 |
| B4-017 | 3PhAOC + NO | → | 1PhAOCD + NO2 | *ARR2* | 7.50E-12 | -290.0 | |
| B4-018 | 3PhAOC + NO2 | → | PhAOCP | *ARR3* | 6.143E-09 | -1.1 | 0.0 |
| B4-019 | 3PhAOC + NO3 | → | 1PhAOCD + NO2 | *ARR2* | 8.90E-12 | 305.0 | |
| B4-020 | 3PhAOC + HO2 | → | 0.65 PhAOCG + 0.15 PhAOCA + 0.20 1PhAOCD + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 | -730.0 | |
| B4-021 | 3PhAOC + MO2 | → | 0.80 1PhAOCD + 0.20 PhAOCA + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 | -508.0 | |
| B4-022 | 1PhAOCD | → | 0.60 PhOCAnhy + 0.60 HO + 0.40 2PhAO + 0.4 CO2 | *ARR1* | 1.00E+06 | | |
| B4-023 | 2PhAO + NO | → | 0.88 1PhAO + 0.88 NO2 + 0.12 PhAON | *ARR2* | 2.7E-12 | -360.0 | |
| B4-024 | 2PhAO + NO3 | → | 1PhAO + NO2 | *ARR2* | 8.90E-12 | 390.0 | |
| B4-025 | 2PhAO + HO2 | → | PhAOH | *ARR2* | 2.623E-13 | -1300.0 | |
| B4-026 | 2PhAO + MO2 | → | 0.60 1PhAO + 0.20 PhAOO + 0.20 PhAOD + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 | -1038.0 | |
| B4-027 | 1PhAO | → | PhAOD + HO2 | *ARR2(O2)* | 2.50E-14 | 300.0 | |
| B4-028 | 1PhAO | → | PhAD + CH2O + HO2 | *ARR3* | 1.12E+09 | 1.7 | 5233.0 |
| B4-029 | 3PhOCD + NO | → | 1PhDOCD + NO2 | *ARR2* | 7.50E-12 | -290.0 | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| B4-030 | 3PhOCD + NO2 | → | PhPOCD | *ARR3* | 6.143E-09 | -1.1 | 0.0 |
| B4-031 | 3PhOCD + NO3 | → | 1PhDOCD + NO2 | *ARR2* | 8.90E-12 | 305.0 | |
| B4-032 | 3PhOCD + HO2 | → | 0.65 PhGOCD + 0.15 PhAOCD + 0.20 1PhDOCD + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 | -730.0 | |
| B4-033 | 3PhOCD + MO2 | → | 0.80 1PhDOCD + 0.20 PhAOCD + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 | -508.0 | |
| B4-034 | 1PhDOCD | → | 0.60 PhOCAnhy + 0.60 HO2 + 0.40 3PhOC + 0.40 CO2 | *ARR1* | 1.00E+06 | | |
| B4-035 | 3PhOC + NO | → | 1PhOCD + NO2 | *ARR2* | 7.50E-12 | -290.0 | |
| B4-036 | 3PhOC + NO2 | → | PhOCP | *ARR3* | 6.143E-09 | -1.1 | 0.0 |
| B4-037 | 3PhOC + NO3 | → | 1PhOCD + NO2 | *ARR2* | 8.90E-12 | 305.0 | |
| B4-038 | 3PhOC + HO2 | → | 0.65 PhOCG + 0.15 PhOCA + 0.20 1PhOCD + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 | -730.0 | |
| B4-039 | 3PhOC + MO2 | → | 0.80 1PhOCD + 0.20 PhOCA + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 | -508.0 | |
| B4-040 | 1PhOCD | → | 2PhO + CO2 | *ARR1* | 1.00E+06 | | |
| B4-041 | 2PhO + NO | → | 0.88 1PhO + 0.88 NO2 + 0.12 PhON | *ARR2* | 2.7E-12 | -360.0 | |
| B4-042 | 2PhO + NO3 | → | 1PhO + NO2 | *ARR2* | 8.90E-12 | 390.0 | |
| B4-043 | 2PhO + HO2 | → | PhOH | *ARR2* | 2.623E-13 | -1300.0 | |
| B4-044 | 2PhO + MO2 | → | 0.60 1PhO + 0.20 PhOO + 0.20 PhOD + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 | -1038.0 | |
| B4-045 | 1PhO | → | PhOD + HO2 | *ARR2(O2)* | 2.50E-14 | 300.0 | |
| B4-046 | 1PhO | → | PhD + CH2O + HO2 | *ARR3* | 1.12E+09 | 1.7 | 5233.0 |
| B4-047 | PhOCAnhy | → | PhAOCA | *ARR1(H2O)* | 2.50E-22 | | |
| ***BLOCK 5.0: NaO CHEMISTRY*** | | | | | | | |
| B5.0-001 | NaO + HO | → | 0.217 NaOO + 0.217 HO2 + 0.022 ONaO + 0.022 HO2 + 0.044 1Na + 0.065 2ONaO + 0.652 2NaOO | *ARR1* | 1.35E-10 | | |
| B5.0-002 | 2ONaO | → | 0.100 4ONaOBp + 0.162 2ONaOpar + 0.738 2ONaOort | *ARR1* | 1.0E+06 | | |
| B5.0-003 | 2NaOO | → | 0.125 4NaOOBp + 0.375 NaOKort + 0.375 HO2 + 0.500 2NaOOort | *ARR1* | 1.0E+06 | | |
| ***BLOCK 5.1: 4ONaOBp CHEMISTRY (PREROXY BRIDGE)*** | | | | | | | |
| B5.1-001 | 4ONaOBp | → | 0.75 2ONaOBp + 0.25 1ONaEpox | *ARR1* | 1.0E+06 | | |
| B5.1-002 | 2ONaOBp + NO | → | 0.91 1ONaOBp + 0.09 ONaONBp + 0.91 NO2 | *ARR2* | 2.7E-12 | -360.0 | |
| B5.1-003 | 2ONaOBp + HO2 | → | ONaOHBp | *ARR2* | 2.447E-13 | -1300.0 | |
| B5.1-004 | 2ONaOBp + NO3 | → | 1ONaOBp + NO2 | *ARR2* | 8.90E-12 | 390.0 | |
| B5.1-005 | 2ONaOBp + MO2 | → | 0.60 1ONaOBp + 0.20 ONaOOBp + 0.20 ONaOKBp + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 | -598.0 | |
| B5.1-006 | 1ONaOBp | → | 1OPhDOD | *ARR3* | 1.12E+09 | 1.7 | 2413.0 |
| B5.1-007 | 1OPhDOD | → | GLYOX + OPhDD + HO2 | *ARR3* | 1.12E+09 | 1.7 | 1644.0 |
| B5.1-008 | 1ONaEpox | → | 1OPhDEnol | *ARR3* | 1.12E+09 | 1.7 | 2301.0 |
| B5.1-009 | 1OPhDEnol | → | OPhDD + 2DC | *ARR3* | 1.12E+09 | 1.7 | 4830.9 |
| ***BLOCK 5.2: 2ONaOpar CHEMISTRY (PARA RO2)*** | | | | | | | |
| B5.2-001 | 2ONaOpar + NO | → | 0.82 1ONaOpar + 0.18 ONaONpar + 0.82 NO2 | *ARR2* | 2.7E-12 | -360.0 | |
| B5.2-002 | 2ONaOpar + HO2 | → | ONaOHpar | *ARR2* | 2.577E-13 | -1300.0 | |
| B5.2-003 | 2ONaOpar + NO3 | → | 1ONaOpar + NO2 | *ARR2* | 8.90E-12 | 390.0 | |
| B5.2-004 | 2ONaOpar + MO2 | → | 0.60 1ONaOpar + 0.20 ONaOOpar + 0.20 ONaOKpar + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.00E-13 | -663.59 | |
| B5.2-005 | 1ONaOpar | → | ONaOKpar + HO2 | *ARR1(O2)* | 2.50E-14 | 300.0 | |
| B5.2-006 | ONaOKpar + HO | → | 0.225 ONaQuin + 0.775 2ONaOOK + 0.225 HO2 | *ARR1* | 8.80E-11 | | |
| B5.2-007 | 2ONaOOK + NO | → | 0.875 1ONaOOK + 0.125 ONaNOOK + 0.875 NO2 | *ARR2* | 2.7E-12 | -360.0 | |
| B5.2-008 | 2ONaOOK + HO2 | → | ONaHOOK | *ARR2* | 2.659E-13 | -1300.0 | |
| B5.2-009 | 2ONaOOK + NO3 | → | 1ONaOOK + NO2 | *ARR2* | 8.90E-12 | 390.0 | |
| B5.2-010 | 2ONaOOK + MO2 | → | 0.60 1ONaOOK + 0.20 ONaOOOK + 0.20 ONaOOKK + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 | -791.0 | |
| B5.2-011 | 1NaOOK | → | OPhODKD + HO2 | *ARR3* | 1.12E+09 | 1.7 | 2301.0 |

***BLOCK 5.3: 2ONaOort CHEMISTRY (ORTHO RO2)***

| | | | | | |
|---|---|---|---|---|---|
| B5.3-001 | 2ONaOort + NO | → | 0.875 1ONaOort + 0.125 ONaONort + 0.875 NO2 | *ARR2* | 2.7E-12 -360.0 |
| B5.3-002 | 2ONaOort + HO2 | → | ONaOHort | *ARR2* | 2.659E-13 -1300.0 |
| B5.3-003 | 2ONaOort + NO3 | → | 1ONaOort + NO2 | *ARR2* | 8.90E-12 390.0 |
| B5.3-004 | 2ONaOort + MO2 | → | 0.60 1ONaOort + 0.20 ONaOOort + 0.20 ONaOKort + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -791.0 |
| B5.3-005 | 2ONaOort | → | ONaOPEN + HO | *ARR2* | 1.90E11 9750.0 |
| B5.3-006 | 1ONaOort | → | ONaOPEN + HO2 | *ARR3* | 1.12E+09 1.7 2301.0 |
| B5.3-007 | ONaOPEN + HO | → | 0.52 2OPhDOD + 0.48 4ONaOPEN | *ARR1* | 6.50E-11 |
| B5.3-008 | ONaOPEN | → | 3OPhU + CO + HO2 | *PHOTO* | 2.2690E-05 |
| B5.3-009 | ONaOPEN | → | OPhDD + 2.0 CO + 2.0 HO2 | *PHOTO* | 6.4685E-06 |
| B5.3-010 | ONaOPEN | → | 5OPhDCrg + CO | *PHOTO* | 6.2783E-06 |
| B5.3-011 | ONaOPEN | → | 4ONaOPEN + HO2 | *PHOTO* | 6.2783E-06 |
| B5.3-012 | 5OPhDCrg | → | 0.625 OPhDCA + 0.375 OPhDCD + 0.375 H2O2 | *ARR1(H2O)* | 1.205E-14 |
| B5.3-013 | 5OPhDCrg | → | OPhDCD + HO | *ARR1* | 0.114E+03 |
| B5.3-014 | 2OPhDOD + NO | → | 0.810 1OPhDOD + 0.190 OPhDNOD + 0.810 NO2 | *ARR2* | 2.7E-12 -360.0 |
| B5.3-015 | 2OPhDOD + NO3 | → | 1OPhDOD + NO2 | *ARR2* | 8.90E-12 390.0 |
| B5.3-016 | 2OPhDOD + HO2 | → | OPhDHOD | *ARR2* | 2.66E-13 -1300.0 |
| B5.3-017 | 2OPhDOD + MO2 | → | 0.60 1OPhDOD + 0.20 OPhDOOD + 0.20 OPhDKOD + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -1031.0 |
| B5.3-018 | 2OPhDOD + HO | → | 1OPhDOD + HO2 | *ARR2* | 3.70E-11 -350.0 |
| B5.3-019 | 4ONaOPEN | → | 0.40 2OPhUEst + 0.60 3OPhUD | *ARR1* | 1.00E+06 |
| B5.3-020 | 2OPhUEst + NO | → | 1OPhUEst + NO2 | *ARR2* | 2.7E-12 -360.0 |
| B5.3-021 | 2OPhUEst + HO2 | → | 0.460 OPhUAnhy + 0.20 HO + 0.20 HO2 | *ARR2* | 2.62E-13 -1300.0 |
| B5.3-022 | 2OPhUEst + NO3 | → | 1OPhUEst + NO2 | *ARR2* | 8.90E-12 390.0 |
| B5.3-023 | 2OPhUEst + MO2 | → | 0.60 1OPhUEst + 0.20 OPhUAnhy + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -955.0 |
| B5.3-024 | 1OPhUEst | → | OPhUAnhy + HO2 | *ARR2(O2)* | 2.5E-14 300.0 |
| B5.3-025 | 1OPhUEst | → | 3OPhUA | *ARR3* | 8.00E+10 1.7 3723.0 |
| B5.3-026 | 3OPhUA + NO | → | 1OPhDUA + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B5.3-027 | 3OPhUA + NO2 | → | | *ARR3* | 6.143E-09 -1.1 0.0 |
| B5.3-028 | 3OPhUA + NO3 | → | 1OPhDUA + NO2 | *ARR2* | 8.90E-12 305.0 |
| B5.3-029 | 3OPhUA + HO2 | → | 0.15 OPhAUA + 0.20 1OPhDUA + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 -730.0 |
| B5.3-030 | 3OPhUA + MO2 | → | 0.80 1OPhDUA + 0.20 OPhAUA + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B5.3-031 | 3OPhUD + NO | → | 1OPhDUD + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B5.3-032 | 3OPhUD + NO2 | → | | *ARR3* | 6.143E-09 -1.1 0.0 |
| B5.3-033 | 3OPhUD + NO3 | → | 1OPhDUD + NO2 | *ARR2* | 8.90E-12 305.0 |
| B5.3-034 | 3OPhUD + HO2 | → | 0.20 1OPhDUD + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 -730.0 |
| B5.3-035 | 3OPhUD + MO2 | → | 0.80 1OPhDUD + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B5.3-036 | 1OPhDUA | → | 0.60 OPhUAnhy + 0.60 HO + 0.23 OPhAD + 0.23 CO2 + 0.23 CO + 0.23 HO2 + 0.17 2OPhUA + 0.17 CO2 | *ARR1* | 1.00E+06 |
| B5.3-037 | 1OPhDUD | → | 0.60 OPhUAnhy + 0.60 HO2 + 0.23 3OPhU + 0.23 CO2 + 0.17 OPhDD + 0.17 CO + 0.17 CO2 + 0.17 HO2 | *ARR1* | 1.00E+06 |
| B5.3-038 | 3OPhU + NO | → | 1OPhUD + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B5.3-039 | 3OPhU + NO3 | → | 1OPhUD + NO2 | *ARR2* | 8.90E-12 305.0 |
| B5.3-040 | 3OPhU + HO2 | → | 0.20 1OPhUD + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 -730.0 |
| B5.3-041 | 3OPhU + MO2 | → | 0.80 1OPhUD + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B5.3-042 | 1OPhUD | → | OPhD + CO + CO2 + HO2 | *ARR1* | 1.00E+06 |
| B5.3-043 | 2OPhUA + NO | → | 1OPhUA + NO2 | *ARR2* | 2.7E-12 -360.0 |
| B5.3-044 | 2OPhUA + NO2 | → | 1OPhUA + NO3 | *ARR3* | 6.143E-09 -1.1 0.0 |
| B5.3-045 | 2OPhUA + NO3 | → | 1OPhUA + NO2 | *ARR2* | 8.90E-12 390.0 |
| B5.3-046 | 2OPhUA + HO2 | → | OHPhUA | *ARR2* | 2.335E-13 -1300.0 |
| B5.3-047 | 2OPhUA + MO2 | → | 0.80 1OPhUA + 0.20 OOPhUA + CH2O + 0.80 HO2 | *ARR2* | 1.03E-13 -398.0 |
| B5.3-048 | 1OPhUA + O3 | → | 2OPhUA | *ARR1* | 2.86E-13 |
| B5.3-049 | 1OPhUA + NO2 | → | VOOPhUA | *ARR1* | 2.08E-12 |
| B5.3-050 | 1OPhUA + HO2 | → | OOPhUA | *ARR1* | 2.30E-13 |
| B5.3-051 | OPhUAnhy | → | OPhAUA | *ARR1(H2O)* | 2.50E-22 |

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|---|---|---|---|---|---|
| ***BLOCK 5.4: 4NaOOBp CHEMISTRY (PREROXY BRIDGE)*** | | | | | |
| B5.4-001 | 4NaOOBp | → | 0.75 2NaOOBp + 0.25 1NaOEpox | *ARR1* | 1.0E+06 |
| B5.4-002 | 2NaOOBp + NO | → | 0.91 1NaOOBp + 0.09 NaOONBp + 0.91 NO2 | *ARR2* | 2.7E-12 -360.0 |
| B5.4-003 | 2NaOOBp + HO2 | → | NaOOHBp | *ARR2* | 2.447E-13 -1300.0 |
| B5.4-004 | 2NaOOBp + NO3 | → | 1NaOOBp + NO2 | *ARR2* | 8.90E-12 390.0 |
| B5.4-005 | 2NaOOBp + MO2 | → | 0.60 1NaOOBp + 0.20 NaOOOBp + 0.20 NaOOKBp + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -598.0 |
| B5.4-006 | 1NaOOBp | → | 1PhDOOD | *ARR3* | 1.12E+09 1.7 2413.0 |
| B5.4-007 | 1PhDOOD | → | GLYOX + PhAD + HO2 | *ARR3* | 1.12E+09 1.7 1644.0 |
| B5.4-008 | 1NaOEpox | → | 1PhAEnol | *ARR3* | 1.12E+09 1.7 2301.0 |
| B5.4-009 | 1PhAEnol | → | PhAD + 2DC | *ARR3* | 1.12E+09 1.7 4830.9 |
| ***BLOCK 5.5: 2NaOOort CHEMISTRY*** | | | | | |
| B5.5-001 | 2NaOOort + NO | → | 0.875 1NaOOort + 0.125 NaOONort + 0.875 NO2 | *ARR2* | 2.7E-12 -360.0 |
| B5.5-002 | 2NaOOort + HO2 | → | NaOOHort | *ARR2* | 2.659E-13 -1300.0 |
| B5.5-003 | 2NaOOort + NO3 | → | 1NaOOort + NO2 | *ARR2* | 8.90E-12 390.0 |
| B5.5-004 | 2NaOOort + MO2 | → | 0.60 1NaOOort + 0.20 NaOOOort + 0.20 NaOOKort + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -791.0 |
| B5.5-005 | 2NaOOort | → | NaOPENOL + HO | *ARR2* | 1.90E11 9750.0 |
| B5.5-006 | 1NaOOort | → | NaOPENOL + HO2 | *ARR3* | 1.12E+09 1.7 2301.0 |
| B5.5-007 | NaOPENOL + HO | → | 0.33 4NaOPENOL + 0.38 PhDKOD + 0.38 HO2 + 0.22 2PhDKD + 0.07 2PhDOOD | *ARR1* | 9.60E-11 |
| B5.5-008 | 2PhDOOD + NO | → | 0.82 1PhDOOD1 + 0.18 PhDOOND + 0.82 NO2 | *ARR2* | 2.7E-12 -360.0 |
| B5.5-009 | 2PhDOOD + HO2 | → | PhDOOHD | *ARR2* | 2.688E-13 -1300.0 |
| B5.5-010 | 2PhDOOD + NO3 | → | 1PhDOOD1 + NO2 | *ARR2* | 8.90E-12 390.0 |
| B5.5-011 | 2PhDOOD + MO2 | → | 0.60 1PhDOOD1 + 0.20 PhDOOKD + 0.20 PhDOOOD + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -791.0 |
| B5.5-012 | 1PhDOOD1 | → | PhDOOD1 + CO + HO2 | *ARR3* | 1.120E+09 1.7 3572.0 |
| B5.5-013 | PhDOOD1 + HO | → | 0.60 PhOOAnhy + 0.36 HO2 + 0.24 HO + 0.20 PhA + 0.40 CO2 + 0.20 HO2 + 0.12 PhAD + 0.12 CO2 + 0.12 HO2 + 0.08 PhAA + 0.08 CO2 + 0.08 HO2 | *ARR1* | 2.7E-11 |
| B5.5-014 | PhOOAnhy | → | PhAOOA | *ARR1(H2O)* | 2.50E-22 |
| B5.5-015 | 2PhDKD + NO | → | 0.91 1PhDKD + 0.09 PhDKND + 0.91 NO2 | *ARR2* | 2.7E-12 -360.0 |
| B5.5-016 | 2PhDKD + HO2 | → | 0.52 PhDKHD + 0.48 1PhDKD + 0.48 HO | *ARR2* | 2.659E-13 -1300.0 |
| B5.5-017 | 2PhDKD + NO3 | → | 1PhDKD + NO2 | *ARR2* | 8.90E-12 390.0 |
| B5.5-018 | 2PhDKD + MO2 | → | 0.80 1PhDKD + 0.20 PhDKOD + 0.80 HO2 + CH2O | *ARR2* | 1.03E-13 -894.0 |
| B5.5-019 | 1PhDKD | → | 0.50 3PhD + 0.50 GLYOX + 0.50 PhKDD + 0.5 HO2 + 0.5 CO | *ARR3* | 1.120E+09 1.7 4378.0 |
| B5.5-020 | 4NaOPENOL | → | 0.40 2PhOUEst + 0.60 3PhOUD | *ARR1* | 1.00E+06 |
| B5.5-021 | 2PhOUEst + NO | → | 1PhOUEst + NO2 | *ARR2* | 2.7E-12 -360.0 |
| B5.5-022 | 2PhOUEst + HO2 | → | 0.540 PhOUHEst + 0.460 PhOUAnhy + 0.20 HO + 0.20 HO2 | *ARR2* | 2.62E-13 -1300.0 |
| B5.5-023 | 2PhOUEst + NO3 | → | 1PhOUEst + NO2 | *ARR2* | 8.90E-12 390.0 |
| B5.5-024 | 2PhOUEst + MO2 | → | 0.60 1PhOUEst + 0.20 PhOUAnhy + 0.20 PhOUOEst + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -955.0 |
| B5.5-025 | 1PhOUEst | → | PhOUAnhy + HO2 | *ARR2(O2)* | 2.5E-14 300.0 |
| B5.5-026 | 1PhOUEst | → | 3PhOUA | *ARR3* | 8.00E+10 1.7 3723.0 |
| B5.5-027 | 3PhOUA + NO | → | 1PhDOUA + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B5.5-028 | 3PhOUA + NO2 | → | PhPOUA | *ARR3* | 6.143E-09 -1.1 0.0 |
| B5.5-029 | 3PhOUA + NO3 | → | 1PhDOUA + NO2 | *ARR2* | 8.90E-12 305.0 |
| B5.5-030 | 3PhOUA + HO2 | → | 0.65 PhGOUA + 0.15 PhAOUA + 0.20 1PhDOUA + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 -730.0 |
| B5.5-031 | 3PhOUA + MO2 | → | 0.80 1PhDOUA + 0.20 PhAOUA + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B5.5-032 | 3PhOUD + NO | → | 1PhDOUD + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B5.5-033 | 3PhOUD + NO2 | → | PhPOUD | *ARR3* | 6.143E-09 -1.1 0.0 |

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|---|---|---|---|---|---|
| B5.5-034 | 3PhOUD + NO3 | → | 1PhDOUD + NO2 | *ARR2* | 8.90E-12 305.0 |
| B5.5-035 | 3PhOUD + HO2 | → | 0.65 PhGOUD + 0.15 PhAOUD + 0.20 1PhDOUD + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 -730.0 |
| B5.5-036 | 3PhOUD + MO2 | → | 0.80 1PhDOUD + 0.20 PhAOUD + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B5.5-037 | 1PhDOUA | → | 0.60 PhOUAnhy + 0.60 HO + 0.23 PhAA + 0.23 CO2 + 0.23 HO2 + 0.23 CO + 0.17 2PhOUA + 0.17 CO2 | *ARR1* | 1.00E+06 |
| B5.5-038 | 1PhDOUD | → | 0.60 PhOUAnhy + 0.60 HO2 + 0.23 3PhOU + 0.23 CO2 + 0.17 PhAD + 0.17 CO + 0.17 CO2 + 0.17 HO2 | *ARR1* | 1.00E+06 |
| B5.5-039 | 2PhOUA + NO | → | 1PhOUA + NO2 | *ARR2* | 2.7E-12 -360.0 |
| B5.5-040 | 2PhOUA + NO2 | → | 1PhOUA + NO3 | *ARR3* | 6.143E-09 -1.1 0.0 |
| B5.5-041 | 2PhOUA + NO3 | → | 1PhOUA + NO2 | *ARR2* | 8.90E-12 390.0 |
| B5.5-042 | 2PhOUA + HO2 | → | HPhOUA | *ARR2* | 2.335E-13 -1300.0 |
| B5.5-043 | 2PhOUA + MO2 | → | 0.80 1PhOUA + 0.20 OPhOUA + CH2O + 0.80 HO2 | *ARR2* | 1.03E-13 -398.0 |
| B5.5-044 | 1PhOUA + O3 | → | 2PhOUA | *ARR1* | 2.86E-13 |
| B5.5-045 | 1PhOUA + NO2 | → | VOPhOUA | *ARR1* | 2.08E-12 |
| B5.5-046 | 1PhOUA + HO2 | → | OPhOUA | *ARR1* | 2.30E-13 |
| B5.5-047 | 3PhOU + NO | → | 1PhOUD + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B5.5-048 | 3PhOU + NO2 | → | PhOUP | *ARR3* | 6.143E-09 -1.1 0.0 |
| B5.5-049 | 3PhOU + NO3 | → | 1PhOUD + NO2 | *ARR2* | 8.90E-12 305.0 |
| B5.5-050 | 3PhOU + HO2 | → | 0.65 PhOUG + 0.15 PhOUA + 0.20 1PhOUD + 0.15 O3 + 0.20 HO | *ARR2* | 3.324E-12 -730.0 |
| B5.5-051 | 3PhOU + MO2 | → | 0.80 1PhOUD + 0.20 PhOUA + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B5.5-052 | 1PhOUD | → | PhA + HO2 + CO2 + CO | *ARR1* | 1.00E+06 |
| B5.5-053 | PhOUAnhy | → | PhAOUA | *ARR1(H2O)* | 2.50E-22 |

***BLOCK 5.6: NaOKort CHEMISTRY***

| | | | | | |
|---|---|---|---|---|---|
| B5.6-001 | NaOKort + HO | → | 0.215 NaKK + 0.785 2NaOOK2 + 0.215 HO2 | *ARR2* | 1.54E-11 -540.0 |
| B5.6-002 | NaKK + HO | → | 2NaOKK | *ARR2* | 7.075E-12 -540.0 |
| B5.6-003 | 2NaOKK + NO | → | 0.875 1NaOKK + 0.125 NaOKKN + 0.875 NO2 | *ARR2* | 2.7E-12 -360.0 |
| B5.6-004 | 2NaOKK + HO2 | → | NaOKKH | *ARR2* | 2.659E-13 -1300.0 |
| B5.6-005 | 2NaOKK + NO3 | → | 1NaOKK + NO2 | *ARR2* | 8.90E-12 390.0 |
| B5.6-006 | 2NaOKK + MO2 | → | 0.60 1NaOKK + 0.20 NaOOKK + 0.20 NaOKKK + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -894.0 |
| B5.6-007 | 1NaOKK | → | 0.815 PhDKKD + 0.185 3PhO + 0.815 HO2 + 0.37 CO | *ARR3* | 1.120E+09 1.7 2301.70 |
| B5.6-008 | 2NaOOK2 + NO | → | 0.875 1NaOOK2 + 0.125 NaNOOK + 0.875 NO2 | *ARR2* | 2.7E-12 -360.0 |
| B5.6-009 | 2NaOOK2 + HO2 | → | NaHOOK | *ARR2* | 2.659E-13 -1300.0 |
| B5.6-010 | 2NaOOK2 + NO3 | → | 1NaOOK2 + NO2 | *ARR2* | 8.90E-12 390.0 |
| B5.6-011 | 2NaOOK2 + MO2 | → | 0.60 1NaOOK2 + 0.20 NaOOOK + 0.20 NaOOKK + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -791.0 |
| B5.6-012 | 1NaOOK2 | → | 0.322 PhODKD + 0.778 PhDKOD + HO2 | *ARR3* | 1.120E+09 1.7 2301.70 |
| B5.6-013 | NaOKort + NO3 | → | 2NaKON | *ARR1* | 3.04E-13 |
| B5.6-014 | 2NaKON + NO | → | 0.875 1NaKON + 0.125 NaNKON + 0.875 NO2 | *ARR2* | 2.7E-12 -360.0 |
| B5.6-015 | 2NaKON + HO2 | → | NaHKON | *ARR2* | 2.659E-13 -1300.0 |
| B5.6-016 | 2NaKON + NO3 | → | 1NaKON + NO2 | *ARR2* | 8.90E-12 390.0 |
| B5.6-017 | 2NaKON + MO2 | → | 0.60 1NaKON + 0.20 NaOKON + 0.20 NaKKON + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -791.0 |
| B5.6-018 | 1NaKON | → | 0.5 PhNDKD + 0.5 PhDKOD + 0.5 HO2 + 0.5 NO2 | *ARR3* | 1.120E+09 1.7 2301.70 |
| B5.6-019 | PhNDKD + HO | → | 0.5 PhKDD + 0.5 3PhND + CO + 0.5 NO2 | *ARR1* | 2.71E-11 |
| B5.6-020 | PhNDKD + NO3 | → | 0.5 PhKDKD + 0.375 PhKDD + 0.125 3PhND + HNO3 + 0.875 NO2 + 0.5 CO | *ARR1* | 3.17E-14 |
| B5.6-021 | PhNDKD | → | PhKDD + NO2 + CO + HO2 | *PHOTO* | 8.2072E-07 |

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|---|---|---|---|---|---|
| B5.6-022 | PhNDKD | → | PhKDD + CO + NO2 + HO2 | *PHOTO* | 5.6804E-06 |
| B5.6-023 | PhNDKD | → | 3PhND + CO + HO2 | *PHOTO* | 8.1954E-05 |
| B5.6-024 | 3PhND + NO | → | 3PhN + NO2 + CO2 | *ARR2* | 7.50E-12 -290.0 |
| B5.6-025 | 3PhND + HO2 | → | 0.65 PhGND + 0.15 PhAND + 0.20 3PhN + 0.15 O3 + 0.20 CO2 + 0.20 HO | *ARR2* | 3.149E-12 -730.0 |
| B5.6-026 | 3PhND + NO3 | → | 3PhN + NO2 + CO2 | *ARR2* | 8.90E-12 -305.0 |
| B5.6-027 | 3PhND + MO2 | → | 0.80 3PhN + 0.20 PhAND + CH2O + 0.80 CO2 + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B5.6-028 | 3PhND + NO2 | → | PhPND | *ARR3* | 6.143E-09 -1.1 0.0 |
| B5.6-029 | 3PhN + NO | → | PhD + 2.0 NO2 + CO2 | *ARR2* | 7.50E-12 -290.0 |
| B5.6-030 | 3PhN + HO2 | → | 0.50 PhD + 0.13 PhNA + 0.37 PhNG + 0.13 O3 + 0.50 CO2 + 0.50 HO + 0.50 NO2 | *ARR2* | 3.149E-12 -730.0 |
| B5.6-031 | 3PhN + NO3 | → | PhD + 2.0 NO2 + CO2 | *ARR2* | 8.90E-12 -305.0 |
| B5.6-032 | 3PhN + MO2 | → | 0.80 PhD + 0.20 PhNA + CH2O + 0.80 CO2 + 0.80 HO2 + 0.80 NO2 | *ARR2* | 2.000E-12 -508.0 |
| B5.6-033 | 3PhN + NO2 | → | PhNP | *ARR3* | 6.143E-09 -1.1 0.0 |
| ***BLOCK 6: PhDD CHEMISTRY*** | | | | | |
| B6-001 | PhDD + HO | → | 0.40 2PhEst + 0.60 3PhD | *ARR1* | 2.63E-11 |
| B6-002 | PhDD | → | 0.40 2PhEst + 0.60 3PhD + HO2 | *PHOTO* | 5.6804E-06 |
| B6-003 | PhDD | → | 0.40 2PhEst + 0.60 3PhD + HO2 | *PHOTO* | 5.6804E-06 |
| B6-004 | PhAD + HO | → | 3PhA | *ARR1* | 1.38E-11 |
| B6-005 | 2PhEst + NO | → | 1PhEst + NO2 | *ARR2* | 2.7E-12 -360.0 |
| B6-006 | 2PhEst + HO2 | → | 0.540 PhEstH + 0.460 PhAnhy + 0.20 HO + 0.20 HO2 | *ARR2* | 2.62E-13 -1300.0 |
| B6-007 | 2PhEst + NO3 | → | 1PhEst + NO2 | *ARR2* | 8.90E-12 390.0 |
| B6-008 | 2PhEst + MO2 | → | 0.60 1PhEst + 0.20 PhAnhy + 0.20 PhEstO + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -1010.0 |
| B6-009 | 1PhEst | → | 3PhA | *ARR3* | 8.00E+10 1.7 3723.0 |
| B6-010 | 3PhA + NO | → | 1PhDA + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B6-011 | 3PhA + HO2 | → | 0.65 PhGA + 0.15 PhAA + 0.20 1PhDA + 0.15 O3 + 0.20 HO | *ARR2* | 3.149E-12 -730.0 |
| B6-012 | 3PhA + NO3 | → | 1PhDA + NO2 | *ARR2* | 8.90E-12 305.0 |
| B6-013 | 3PhA + MO2 | → | 0.80 1PhDA + 0.20 PhAA + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B6-014 | 3PhA + NO2 | → | PhPA | *ARR3* | 6.143E-09 -1.1 0.0 |
| B6-015 | 1PhDA | → | 0.60 PhAnhy + 0.60 HO + 0.40 2PhA + 0.40 CO2 | *ARR1* | 1.00E+06 |
| B6-016 | 2PhA + NO | → | 1PhA + NO2 | *ARR2* | 2.7E-12 -360.0 |
| B6-017 | 2PhA + HO2 | → | HPhA | *ARR2* | 2.335E-13 -1300.0 |
| B6-018 | 2PhA + NO3 | → | 1PhA + NO2 | *ARR2* | 8.90E-12 390.0 |
| B6-019 | 2PhA + MO2 | → | 0.80 1PhA + 0.20 OPhA + CH2O + 0.80 HO2 | *ARR2* | 1.03E-13 -398.0 |
| B6-020 | 2PhA + NO2 | → | 1PhA + NO3 | *ARR3* | 6.143E-09 -1.1 0.0 |
| B6-021 | 1PhA + O3 | → | 2PhA | *ARR1* | 2.86E-13 |
| B6-022 | 1PhA + NO2 | → | VOPhA | *ARR1* | 2.08E-12 |
| B6-023 | 1PhA + HO2 | → | OPhA | *ARR1* | 2.30E-13 |
| B6-024 | 3PhD + NO | → | 1PhDD + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B6-025 | 3PhD + HO2 | → | 0.65 PhGD + 0.15 PhAD + 0.20 1PhDD + 0.15 O3 + 0.20 HO | *ARR2* | 3.149E-12 -730.0 |
| B6-026 | 3PhD + NO3 | → | 1PhDD + NO2 | *ARR2* | 8.90E-12 -305.0 |
| B6-027 | 3PhD + MO2 | → | 0.80 1PhDD + 0.20 PhAD + CH2O + 0.80 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B6-028 | 3PhD + NO2 | → | PhPD | *ARR3* | 6.143E-09 -1.1 0.0 |
| B6-029 | 1PhDD | → | 0.40 2PhD + 0.60 PhAnhy + 0.40 CO2 + 0.60 HO2 | *ARR1* | 1.00E+06 |
| B6-030 | 2PhD + NO | → | 1PhD + NO2 | *ARR2* | 2.7E-12 -360.0 |
| B6-031 | 2PhD + HO2 | → | HPhD | *ARR2* | 2.335E-13 -1300.0 |
| B6-032 | 2PhD + NO3 | → | 1PhD + NO2 | *ARR2* | 8.90E-12 390.0 |
| B6-033 | 2PhD + MO2 | → | 0.80 1PhD + 0.20 OPhD + CH2O + 0.80 HO2 | *ARR2* | 1.03E-13 -398.0 |
| B6-034 | 2PhD + NO2 | → | 1PhD + NO3 | *ARR3* | 6.143E-09 -1.1 0.0 |
| B6-035 | 1PhD + O3 | → | 2PhD | *ARR1* | 2.86E-13 |
| B6-036 | 1PhD + NO2 | → | VOPhD | *ARR1* | 2.08E-12 |
| B6-037 | 1PhD + HO2 | → | OPhD | *ARR1* | 2.30E-13 |
| B6-038 | PhAnhy | → | PhAA | *ARR1(H2O)* | 2.50E-22 |

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|---|---|---|---|---|---|
| ***BLOCK 7: NaOO CHEMISTRY*** | | | | | |
| B7-001 | NaOO + HO | → | 0.23 NaOOO + 0.23 HO2 + 0.07 1NaO + 0.70 2NaOOO | *ARR1* | 4.955E-10 |
| B7-002 | 1NaO + O3 | → | 2NaO | *ARR1* | 2.86E-13 |
| B7-003 | 1NaO + NO2 | → | NaVOO | *ARR1* | 2.08E-12 |
| B7-004 | 1NaO + HO2 | → | NaOO | *ARR1* | 2.30E-13 |
| B7-005 | 2NaO + NO | → | 1NaO + NO2 | *ARR2* | 2.7E-12 -360.0 |
| B7-006 | 2NaO + NO2 | → | 1NaO + NO3 | *ARR3* | 6.143E-09 -1.1 0.00 |
| B7-007 | 2NaO + NO3 | → | 1NaO + NO2 | *ARR2* | 8.90E-12 390.0 |
| B7-008 | 2NaO + HO2 | → | NaHO | *ARR2* | 2.096E-13 -1300.0 |
| B7-009 | 2NaO + MO2 | → | 0.80 1NaO + 0.20 NaOO + CH2O + 0.80 HO2 | *ARR2* | 1.03E-13 -324.0 |
| B7-010 | 2NaOOO | → | 0.25 NaOOK + 0.25 HO2 + 0.75 2NaOOOBp | *ARR1* | 1.0E+06 |
| B7-011 | 2NaOOOBp | → | NaOOKBp + HO2 | *ARR2* | 5.60E12 6010.0 |
| B7-012 | 2NaOOOBp + NO | → | 0.91 1NaOOOBp + 0.09 NaOOONBp + 0.91 NO2 | *ARR2* | 2.7E-12 -360.0 |
| B7-013 | 2NaOOOBp + HO2 | → | NaOOOHBp | *ARR2* | 2.447E-13 -1300.0 |
| B7-014 | 2NaOOOBp + NO3 | → | 1NaOOOBp + NO2 | *ARR2* | 8.90E-12 390.0 |
| B7-015 | 2NaOOOBp + MO2 | → | 0.80 1NaOOOBp + 0.20 NaOOOOBp + CH2O + 0.80 HO2 | *ARR2* | 1.03E-13 -598.0 |
| B7-016 | 1NaOOOBp | → | 1PhAOOD | *ARR3* | 1.12E+09 1.7 2413.0 |
| B7-017 | 1PhAOOD | → | 0.5 GLYOX + 0.5 PhAA + 0.5 GLYA + 0.5 PhAD + HO2 | *ARR3* | 1.12E+09 1.7 1644.0 |
| ***BLOCK 8: C2 AND C1 CHEMISTRY*** | | | | | |
| B8-001 | 2DC + NO | → | 1DC + NO2 | *ARR2* | 2.7E-12 -360.0 |
| B8-002 | 2DC + HO2 | → | DH | *ARR2* | 1.396E-13 -1300.0 |
| B8-003 | 2DC + NO3 | → | 1DC + NO2 | *ARR2* | 8.90E-12 390.0 |
| B8-004 | 2DC + MO2 | → | 0.60 1DC + 0.20 GLYOX + 0.20 DO + 0.60 HO2 + 0.80 CH2O + 0.20 MOH | *ARR2* | 1.03E-13 -558.0 |
| B8-005 | 1DC | → | CH2O + CO + HO2 | *ARR3* | 1.120E+09 1.7 4730.3 |
| B8-006 | DH + HO | → | 0.21 GLYOX + HO | *ARR1* | 1.32E-11 |
| B8-007 | DO + HO | → | 0.27 GLYOX + HO2 | *ARR1* | 1.02E-11 |
| B8-008 | DO + NO3 | → | GLYOX + HNO3 + HO2 | *ARR1* | 6.84E-14 |
| B8-009 | GLYOX + HO | → | 0.30 3GLY + 1.4 CO + 0.70 HO2 | *ARR2* | 2.17E-12 -340.0 |
| B8-010 | GLYOX + NO3 | → | 0.30 3GLY + HNO3 + 1.4 CO + 0.70 HO2 | *ARR2* | 2.80E-12 2375.0 |
| B8-011 | GLYOX | → | 2.0 CO | *PHOTO* | 1.9242E-06 |
| B8-012 | GLYOX | → | 2.0 CO + 2.0 HO2 | *PHOTO* | 2.9389E-05 |
| B8-013 | GLYOX | → | CH2O + CO | *PHOTO* | 1.0377E-05 |
| B8-014 | 3GLY + NO | → | CO + CO2 + HO2 + NO2 | *ARR2* | 7.50E-12 -290.0 |
| B8-015 | 3GLY + NO2 | → | CO + CO2 + HO2 + NO3 | *ARR3* | 6.143E-09 -1.1 0.0 |
| B8-016 | 3GLY + NO3 | → | CO + CO2 + HO2 + NO2 | *ARR2* | 8.90E-12 305.0 |
| B8-017 | 3GLY + HO2 | → | 0.37 GLYG + 0.13 GLYA + 0.5 CO + 0.5 CO2 + 0.5 HO + 0.5 HO2 + 0.13 O3 | *ARR2* | 2.105E-12 -730.0 |
| B8-018 | 3GLY + MO2 | → | 0.8 CO + 0.8 CO2 + 0.20 GLYA + CH2O + 1.60 HO2 | *ARR2* | 2.000E-12 -508.0 |
| B8-019 | GLYG + HO | → | 0.193 3GLY + 0.807 HO2 + 1.614 CO | *ARR1* | 1.60E-11 |
| B8-020 | GLYG | → | CHOOH + CO2 | *PHOTO* | 3.2745E-04 |
| B8-021 | GLYG | → | CO + CO2 | *PHOTO* | 2.7778E-05 |
| B8-022 | GLYA + HO | → | 2.0 CO + HO | *ARR1* | 1.34E-11 |
| B8-023 | GLYA | → | CH2O + CO2 | *PHOTO* | 3.2745E-04 |
| B8-024 | GLYA | → | 2.0 CO | *PHOTO* | 2.7778E-05 |
| B8-025 | CHOOH + HO | → | CO2 + HO2 | *ARR1* | 4.50E-13 |
| B8-026 | CH2O + HO | → | HO2 + CO | *ARR2* | 8.60E-12 -20.0 |
| B8-027 | CH2O + NO3 | → | HO2 + HNO3 + CO | *ARR2* | 2.00E-12 2440.0 |
| B8-028 | CH2O | → | 2.0 HO2 + CO | *PHOTO* | 1.1868E-05 |
| B8-029 | CH2O | → | CO | *PHOTO* | 4.9249E-05 |
| ***BLOCK 9: LOSS REACTIONS*** | | | | | |
| B9-001 | NaVO + HO | → | | *ARR1* | 2.60E-11 |
| B9-002 | NaH + HO | → | | *ARR1* | 7.80E-11 |
| B9-003 | NaONpar + HO | → | | *ARR1* | 1.34E-10 |
| B9-004 | NaOHpar + O3 | → | | *ARR1* | 1.15E-17 |
| B9-005 | NaONpar + NO3 | → | | *ARR1* | 3.05E-13 |
| B9-006 | NaOHpar + HO | → | | *ARR1* | 1.92E-10 |
| B9-007 | NaOHpar + O3 | → | | *ARR1* | 2.62E-16 |
| B9-008 | NaOHpar + NO3 | → | | *ARR1* | 3.05E-13 |

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|---|---|---|---|---|---|---|
| B9-009 | NaOOpar + HO | → | | *ARR1* | 3.29E-10 | |
| B9-010 | NaOOpar + O3 | → | | *ARR1* | 3.67E-16 | |
| B9-011 | NaOOpar + NO3 | → | | *ARR1* | 2.73E-13 | |
| B9-012 | NaOKpar + O3 | → | | *ARR1* | 5.24E-18 | |
| B9-013 | NaOKpar + NO3 | → | | *ARR1* | 7.96E-15 | |
| B9-014 | NaQuin + HO | → | | *ARR1* | 3.17E-11 | |
| B9-015 | NaNOOK + HO | → | | *ARR1* | 8.13E-12 | |
| B9-016 | NaNOOK + NO3 | → | | *ARR1* | 5.30E-15 | |
| B9-017 | NaHOOK + HO | → | | *ARR1* | 4.11E-11 | |
| B9-018 | NaHOOK + NO3 | → | | *ARR1* | 5.30E-15 | |
| B9-019 | NaOOOK + HO | → | | *ARR1* | 4.93E-11 | |
| B9-020 | NaOOOK + NO3 | → | | *ARR1* | 9.95E-15 | |
| B9-021 | NaOOKK + HO | → | | *ARR1* | 1.13E-11 | |
| B9-022 | NaOOKK + NO3 | → | | *ARR1* | 2.02E-15 | |
| B9-023 | PhOKHEst + HO | → | | *ARR1* | 1.95E-11 | |
| B9-024 | PhOKAnhy + HO | → | | *ARR1* | 6.40E-12 | |
| B9-025 | PhOKOEst + HO | → | | *ARR1* | 1.66E-11 | |
| B9-026 | PhPOKA + HO | → | | *ARR1* | 7.27E-12 | |
| B9-027 | PhPOKA | → | 3PhOKA + NO2 | *ARR2* | 5.20E+16 | 13850.00 |
| B9-028 | PhPOKD + HO | → | | *ARR1* | 1.80E-11 | |
| B9-029 | PhPOKD | → | 3PhOKD + NO2 | *ARR2* | 5.20E+16 | 13850.00 |
| B9-030 | PhGOKD + HO | → | | *ARR1* | 2.59E-11 | |
| B9-031 | PhAOKD + HO | → | | *ARR1* | 2.02E-11 | |
| B9-032 | PhDKA + HO | → | | *ARR1* | 1.23E-11 | |
| B9-033 | HPhOA + HO | → | | *ARR1* | 5.21E-11 | |
| B9-034 | OPhOA + HO | → | | *ARR1* | 1.21E-10 | |
| B9-035 | VOPhOA + HO | → | | *ARR1* | 1.28E-11 | |
| B9-036 | PhOP + HO | → | | *ARR1* | 2.00E-11 | |
| B9-037 | PhOP | → | 3PhO + NO2 | *ARR2* | 5.20E+16 | 13850.00 |
| B9-038 | PhOG + HO | → | | *ARR1* | 2.79E-11 | |
| B9-039 | PhOA + HO | → | | *ARR1* | 2.21E-11 | |
| B9-040 | PhD + HO | → | | *ARR1* | 1.26E-11 | |
| B9-041 | PhKKAnhy + HO | → | | *ARR1* | 1.15E-13 | |
| B9-042 | HPhKA + HO | → | | *ARR1* | 4.42E-12 | |
| B9-043 | OPhKA + HO | → | | *ARR1* | 5.72E-12 | |
| B9-044 | VOPhKA + HO | → | | *ARR1* | 5.16E-13 | |
| B9-045 | PhKP + HO | → | | *ARR1* | 5.01E-13 | |
| B9-046 | PhKP | → | 3PhK + NO2 | *ARR2* | 5.20E+16 | 13850.00 |
| B9-047 | PhKG + HO | → | | *ARR1* | 3.60E-12 | |
| B9-048 | PhKA + HO | → | | *ARR1* | 6.21E-13 | |
| B9-049 | HPh + HO | → | | *ARR1* | 8.32E-12 | |
| B9-050 | OPh + HO | → | | *ARR1* | 2.82E-11 | |
| B9-051 | OPh + NO3 | → | | *ARR1* | 4.50E-12 | |
| B9-052 | VOPh + HO | → | | *ARR1* | 1.64E-12 | |
| B9-053 | PhKAKA + HO | → | | *ARR1* | 3.55E-13 | |
| B9-054 | PhKOHEst + HO | → | | *ARR1* | 1.95E-11 | |
| B9-055 | PhKOAnhy + HO | → | | *ARR1* | 6.40E-12 | |
| B9-056 | PhKOOEst + HO | → | | *ARR1* | 1.66E-11 | |
| B9-057 | PhPKOA + HO | → | | *ARR1* | 2.42E-12 | |
| B9-058 | PhPKOA | → | 3PhKOA + NO2 | *ARR2* | 5.20E+16 | 13850.00 |
| B9-059 | PhPKOD + HO | → | | *ARR1* | 1.94E-11 | |
| B9-060 | PhPKOD | → | 3PhKOD + NO2 | *ARR2* | 5.20E+16 | 13850.00 |
| B9-061 | PhPKOD + NO3 | → | | *ARR1* | 1.85E-13 | |
| B9-062 | PhGKOD + HO | → | | *ARR1* | 2.25E-11 | |
| B9-063 | PhGKOD + NO3 | → | | *ARR1* | 1.85E-13 | |
| B9-064 | PhAKOD + HO | → | | *ARR1* | 2.00E-11 | |
| B9-065 | PhAKOD + NO3 | → | | *ARR1* | 1.85E-13 | |
| B9-066 | PhAKD + HO | → | | *ARR1* | 1.46E-11 | |
| B9-067 | OPhKOA + HO | → | | *ARR1* | 8.43E-12 | |
| B9-068 | PhKOP | → | 3PhKO + NO2 | *ARR2* | 5.20E+16 | 13850.00 |
| B9-069 | PhKOP + HO | → | | *ARR1* | 1.18E-12 | |
| B9-070 | PhKOG + HO | → | | *ARR1* | 9.10E-12 | |
| B9-071 | PhKOA + HO | → | | *ARR1* | 3.34E-12 | |
| B9-072 | PhKD + HO | → | | *ARR1* | 1.34E-11 | |
| B9-073 | HPhKKA + HO | → | | *ARR1* | 4.42E-12 | |
| B9-074 | OPhKKA + HO | → | | *ARR1* | 5.72E-12 | |
| B9-075 | VOPhKKA + HO | → | | *ARR1* | 5.16E-13 | |
| B9-076 | PhKAnhy + HO | → | | *ARR1* | 3.12E-13 | |

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|---|---|---|---|---|---|---|---|
| B9-077 | NaONort + HO | → | | *ARR1* | 9.16E-11 | | |
| B9-078 | NaONort + O3 | → | | *ARR1* | 8.24E-18 | | |
| B9-079 | NaONort + NO3 | → | | *ARR1* | 3.43E-13 | | |
| B9-080 | NaOHort + HO | → | | *ARR1* | 2.26E-10 | | |
| B9-081 | NaOHort + O3 | → | | *ARR1* | 1.87E-16 | | |
| B9-082 | NaOHort + NO3 | → | | *ARR1* | 3.43E-13 | | |
| B9-083 | NaOOort + HO | → | | *ARR1* | 2.65E-10 | | |
| B9-084 | NaOOort + O3 | → | | *ARR1* | 2.62E-16 | | |
| B9-085 | NaOOort + NO3 | → | | *ARR1* | 3.09E-13 | | |
| B9-086 | PhDCD + HO | → | | *ARR1* | 4.06E-11 | | |
| B9-087 | PhDCA + HO | → | | *ARR1* | 1.99E-11 | | |
| B9-088 | PhDNOD + HO | → | | *ARR1* | 2.87E-11 | | |
| B9-089 | PhDNOD + NO3 | → | | *ARR1* | 4.55E-13 | | |
| B9-090 | PhDHOD + HO | → | | *ARR1* | 5.09E-11 | | |
| B9-091 | PhDHOD + NO3 | → | | *ARR1* | 4.55E-13 | | |
| B9-092 | PhDOOD + HO | → | | *ARR1* | 6.03E-11 | | |
| B9-093 | PhDOOD + NO3 | → | | *ARR1* | 4.58E-13 | | |
| B9-094 | PhUAnhy + HO | → | | *ARR2* | 0.622E-11 | -540.0 | |
| B9-095 | PhUAnhy + O3 | → | | *ARR1* | 1.80E-16 | | |
| B9-096 | PhUAnhy + NO3 | → | | *ARR1* | 0.272E-14 | | |
| B9-097 | PhUHEst1 + HO | → | 0.5 PhUAnhy | *ARR1* | 1.17E-10 | | |
| B9-098 | PhUHEst1 + O3 | → | | *ARR1* | 9.00E-15 | | |
| B9-099 | PhUHEst1 + NO3 | → | | *ARR1* | 3.40E-13 | | |
| B9-100 | PhUOEst1 + HO | → | 0.5 PhUAnhy | *ARR1* | 1.25E-10 | | |
| B9-101 | PhUOEst1 + O3 | → | | *ARR1* | 1.26E-14 | | |
| B9-102 | PhUOEst1 + NO3 | → | | *ARR1* | 3.05E-13 | | |
| B9-103 | PhPUA1 + HO | → | | *ARR1* | 5.17E-11 | | |
| B9-104 | PhPUA1 | → | 3PhUA1 + NO2 | *ARR2* | 5.20E+16 | 13850.00 | |
| B9-105 | PhGUA1 + HO | → | 0.1 3PhUA1 | *ARR1* | 5.48E-11 | | |
| B9-106 | PhGUA1 + NO3 | → | | *ARR1* | 3.40E-13 | | |
| B9-107 | PhAUA + HO | → | | *ARR1* | 5.23E-11 | | |
| B9-108 | PhAUA + NO3 | → | | *ARR1* | 3.40E-13 | | |
| B9-109 | PhPUD1 + HO | → | | *ARR1* | 5.87E-11 | | |
| B9-110 | PhPUD1 | → | 3PhUD1 + NO2 | *ARR2* | 5.20E+16 | 13850.00 | |
| B9-111 | PhGUD1 + HO | → | 0.1 3PhUD1 | *ARR1* | 6.18E-11 | | |
| B9-112 | PhAUD1 + HO | → | 0.25 3PhUA1 | *ARR1* | 5.92E-11 | | |
| B9-113 | PhUP | → | 3PhU + NO2 | *ARR2* | 5.20E+16 | 13850.00 | |
| B9-114 | PhUP + HO | → | | *ARR1* | 4.39E-11 | | |
| B9-115 | PhUG + HO | → | | *ARR1* | 4.70E-11 | | |
| B9-116 | PhUG + NO3 | → | | *ARR1* | 3.40E-13 | | |
| B9-117 | PhUA + HO | → | | *ARR1* | 4.45E-11 | | |
| B9-118 | PhUA + NO3 | → | | *ARR1* | 3.40E-13 | | |
| B9-119 | PhUHEst2 + HO | → | 0.5 PhUAnhy | *ARR1* | 1.17E-10 | | |
| B9-120 | PhUHEst2 + O3 | → | | *ARR1* | 9.00E-15 | | |
| B9-121 | PhUHEst2 + NO3 | → | | *ARR1* | 3.40E-13 | | |
| B9-122 | PhUOEst2 + HO | → | 0.5 PhUAnhy | *ARR1* | 1.25E-10 | | |
| B9-123 | PhUOEst2 + O3 | → | | *ARR1* | 1.26E-14 | | |
| B9-124 | PhUOEst2 + NO3 | → | | *ARR1* | 3.05E-13 | | |
| B9-125 | PhPUA2 + HO | → | | *ARR1* | 5.17E-11 | | |
| B9-126 | PhPUA2 | → | 3PhUA2 + NO2 | *ARR2* | 5.20E+16 | 13850.00 | |
| B9-127 | PhGUA2 + HO | → | 0.1 3PhUA2 | *ARR1* | 5.48E-11 | | |
| B9-128 | PhGUA2 + NO3 | → | | *ARR1* | 3.40E-13 | | |
| B9-129 | HPhUA + HO | → | | *ARR1* | 6.18E-11 | | |
| B9-130 | OPhUA + HO | → | | *ARR1* | 1.01E-10 | | |
| B9-131 | VOPhUA + HO | → | | *ARR1* | 7.00E-11 | | |
| B9-132 | PhPUD2 + HO | → | | *ARR1* | 5.87E-11 | | |
| B9-133 | PhPUD2 | → | 3PhUD2 + NO2 | *ARR2* | 5.20E+16 | 13850.00 | |
| B9-134 | PhGUD2 + HO | → | 0.1 3PhUD2 | *ARR1* | 6.18E-11 | | |
| B9-135 | PhAUD2 + HO | → | 0.25 3PhUA2 | *ARR1* | 5.92E-11 | | |
| B9-136 | NaONBp + HO | → | | *ARR1* | 5.38E-11 | | |
| B9-137 | NaONBp + NO3 | → | | *ARR1* | 1.91E-13 | | |
| B9-138 | NaOHBp + HO | → | | *ARR1* | 7.27E-11 | | |
| B9-139 | NaOHBp + NO3 | → | | *ARR1* | 1.91E-13 | | |
| B9-140 | NaOOBp + HO | → | | *ARR1* | 1.04E-10 | | |
| B9-141 | NaOOBp + NO3 | → | | *ARR1* | 2.08E-13 | | |
| B9-142 | NaOKBp + HO | → | | *ARR1* | 2.70E-11 | | |
| B9-143 | NaOKBp + NO3 | → | | *ARR1* | 1.89E-13 | | |
| B9-144 | PhOCHEst + HO | → | | *ARR1* | 3.67E-11 | | |

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|---|---|---|---|---|---|---|
| B9-145 | PhOCAnhy + HO | → | | *ARR1* | 2.52E-11 | |
| B9-146 | PhOCOEst + HO | → | | *ARR1* | 3.67E-11 | |
| B9-147 | PhAOCP | → | 3PhAOC + NO2 | *ARR2* | 5.20E+16 | 13850.00 |
| B9-148 | PhAOCP + HO | → | | *ARR1* | 5.43E-11 | |
| B9-149 | PhAOCG + HO | → | | *ARR1* | 5.93E-11 | |
| B9-150 | PhAOCA + HO | → | | *ARR1* | 6.28E-11 | |
| B9-151 | PhAON + HO | → | | *ARR1* | 4.91E-11 | |
| B9-152 | PhAOH + HO | → | | *ARR1* | 6.28E-11 | |
| B9-153 | PhAOO + HO | → | | *ARR1* | 6.90E-11 | |
| B9-154 | PhAOD + HO | → | | *ARR1* | 6.50E-11 | |
| B9-155 | PhAOD + NO3 | → | | *ARR1* | 2.74E-13 | |
| B9-156 | PhPOCD | → | 3PhOCD + NO2 | *ARR2* | 5.20E+16 | 13850.00 |
| B9-157 | PhPOCD + HO | → | | *ARR1* | 7.57E-11 | |
| B9-158 | PhGOCD + HO | → | | *ARR1* | 7.88E-11 | |
| B9-159 | PhAOCD + HO | → | | *ARR1* | 7.62E-11 | |
| B9-160 | PhOCP | → | 3PhOC + NO2 | *ARR2* | 5.20E+16 | 13850.00 |
| B9-161 | PhOCP + HO | → | | *ARR1* | 2.69E-11 | |
| B9-162 | PhOCG + HO | → | | *ARR1* | 3.19E-11 | |
| B9-163 | PhOCA + HO | → | | *ARR1* | 3.53E-11 | |
| B9-164 | PhON + HO | → | | *ARR1* | 2.16E-11 | |
| B9-165 | PhOH + HO | → | | *ARR1* | 3.54E-11 | |
| B9-166 | PhOO + HO | → | | *ARR1* | 4.15E-11 | |
| B9-167 | PhOD + HO | → | | *ARR1* | 3.75E-11 | |
| B9-168 | PhOD + NO3 | → | | *ARR1* | 2.74E-13 | |
| B9-169 | ONaONBp + HO | → | | *ARR1* | 1.17E-10 | |
| B9-170 | ONaONBp + NO3 | → | | *ARR1* | 1.91E-13 | |
| B9-171 | ONaOHBp + HO | → | | *ARR1* | 1.36E-10 | |
| B9-172 | ONaOHBp + NO3 | → | | *ARR1* | 1.91E-13 | |
| B9-173 | ONaOOBp + HO | → | | *ARR1* | 3.31E-10 | |
| B9-174 | ONaOOBp + NO3 | → | | *ARR1* | 2.08E-13 | |
| B9-175 | ONaOKBp + HO | → | | *ARR1* | 3.54E-11 | |
| B9-176 | ONaOKBp + NO3 | → | | *ARR1* | 1.89E-13 | |
| B9-177 | OPhDD + HO | → | | *ARR1* | 2.43E-11 | |
| B9-178 | ONaONpar + HO | → | | *ARR1* | 3.61E-10 | |
| B9-179 | ONaOHpar + O3 | → | | *ARR1* | 1.15E-17 | |
| B9-180 | ONaONpar + NO3 | → | | *ARR1* | 3.05E-13 | |
| B9-181 | ONaOHpar + HO | → | | *ARR1* | 4.19E-10 | |
| B9-182 | ONaOHpar + O3 | → | | *ARR1* | 2.62E-16 | |
| B9-183 | ONaOHpar + NO3 | → | | *ARR1* | 3.05E-13 | |
| B9-184 | ONaOOpar + HO | → | | *ARR1* | 1.16E-09 | |
| B9-185 | ONaOOpar + O3 | → | | *ARR1* | 3.67E-16 | |
| B9-186 | ONaOOpar + NO3 | → | | *ARR1* | 2.73E-13 | |
| B9-187 | ONaOKpar + O3 | → | | *ARR1* | 5.24E-18 | |
| B9-188 | ONaOKpar + NO3 | → | | *ARR1* | 7.96E-15 | |
| B9-189 | ONaQuin + HO | → | | *ARR1* | 3.49E-11 | |
| B9-190 | ONaNOOK + HO | → | | *ARR1* | 3.23E-11 | |
| B9-191 | ONaNOOK + NO3 | → | | *ARR1* | 5.30E-15 | |
| B9-192 | ONaHOOK + HO | → | | *ARR1* | 6.11E-11 | |
| B9-193 | ONaHOOK + NO3 | → | | *ARR1* | 5.30E-15 | |
| B9-194 | ONaOOOK + HO | → | | *ARR1* | 7.35E-11 | |
| B9-195 | ONaOOOK + NO3 | → | | *ARR1* | 9.95E-15 | |
| B9-196 | ONaOOKK + HO | → | | *ARR1* | 3.55E-11 | |
| B9-197 | ONaOOKK + NO3 | → | | *ARR1* | 2.02E-15 | |
| B9-198 | OPhODKD + HO | → | | *ARR1* | 3.56E-11 | |
| B9-199 | OPhODKD + NO3 | → | | *ARR1* | 2.87E-13 | |
| B9-200 | ONaONort + HO | → | | *ARR1* | 3.40E-10 | |
| B9-201 | ONaONort + O3 | → | | *ARR1* | 8.24E-18 | |
| B9-202 | ONaONort + NO3 | → | | *ARR1* | 3.43E-13 | |
| B9-203 | ONaOHort + HO | → | | *ARR1* | 4.75E-10 | |
| B9-204 | ONaOHort + O3 | → | | *ARR1* | 1.87E-16 | |
| B9-205 | ONaOHort + NO3 | → | | *ARR1* | 3.43E-13 | |
| B9-206 | ONaOOort + HO | → | | *ARR1* | 5.14E-10 | |
| B9-207 | ONaOOort + O3 | → | | *ARR1* | 2.62E-16 | |
| B9-208 | ONaOOort + NO3 | → | | *ARR1* | 3.09E-13 | |
| B9-209 | ONaOKort + HO | → | | *ARR1* | 3.55E-10 | |
| B9-210 | ONaOKort + O3 | → | | *ARR1* | 3.74E-18 | |
| B9-211 | ONaOKort + NO3 | → | | *ARR1* | 8.03E-15 | |
| B9-212 | OPhDCD + HO | → | | *ARR1* | 4.90E-11 | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| B9-213 | OPhDCA + HO | → | | *ARR1* | 2.83E-11 | | |
| B9-214 | OPhDNOD + HO | → | | *ARR1* | 6.00E-11 | | |
| B9-215 | OPhDNOD + NO3 | → | | *ARR1* | 4.66E-14 | | |
| B9-216 | OPhDHOD + HO | → | | *ARR1* | 7.09E-11 | | |
| B9-217 | OPhDHOD + NO3 | → | | *ARR1* | 4.55E-13 | | |
| B9-218 | OPhDOOD + HO | → | | *ARR1* | 8.45E-11 | | |
| B9-219 | OPhDOOD + NO3 | → | | *ARR1* | 4.58E-13 | | |
| B9-220 | OPhDKOD + HO | → | | *ARR1* | 7.20E-11 | | |
| B9-221 | OPhDKOD + NO3 | → | | *ARR1* | 1.34E-14 | | |
| B9-222 | OPhUAnhy + HO | → | | *ARR2* | 0.622E-11 | -540.0 | |
| B9-223 | OPhUAnhy + NO3 | → | | *ARR1* | 0.272E-14 | | |
| B9-224 | OPhAUA + HO | → | | *ARR1* | 5.23E-11 | | |
| B9-225 | OPhAUA + NO3 | → | | *ARR1* | 3.40E-13 | | |
| B9-226 | OPhAD + HO | → | | *ARR1* | 1.38E-11 | | |
| B9-227 | OPhD + HO | → | | *ARR1* | 1.46E-11 | | |
| B9-228 | OHPhUA + HO | → | | *ARR1* | 6.18E-11 | | |
| B9-229 | OOPhUA + HO | → | | *ARR1* | 1.01E-10 | | |
| B9-230 | VOOPhUA + HO | → | | *ARR1* | 7.00E-11 | | |
| B9-231 | NaOONBp + HO | → | | *ARR1* | 8.11E-11 | | |
| B9-232 | NaOONBp + NO3 | → | | *ARR1* | 9.09E-13 | | |
| B9-233 | NaOOHBp + HO | → | | *ARR1* | 9.41E-11 | | |
| B9-234 | NaOOHBp + NO3 | → | | *ARR1* | 9.09E-13 | | |
| B9-235 | NaOOOBp + HO | → | | *ARR1* | 2.16E-10 | | |
| B9-236 | NaOOOBp + NO3 | → | | *ARR1* | 9.26E-13 | | |
| B9-237 | NaOOKBp + HO | → | | *ARR1* | 2.64E-11 | | |
| B9-238 | NaOOKBp + NO3 | → | | *ARR1* | 9.07E-13 | | |
| B9-239 | NaOONort + HO | → | | *ARR1* | 9.16E-11 | | |
| B9-240 | NaOONort + O3 | → | | *ARR1* | 8.24E-18 | | |
| B9-241 | NaOONort + NO3 | → | | *ARR1* | 3.43E-13 | | |
| B9-242 | NaOOHort + HO | → | | *ARR1* | 2.26E-10 | | |
| B9-243 | NaOOHort + O3 | → | | *ARR1* | 1.87E-16 | | |
| B9-244 | NaOOHort + NO3 | → | | *ARR1* | 3.43E-13 | | |
| B9-245 | NaOOOort + HO | → | | *ARR1* | 2.65E-10 | | |
| B9-246 | NaOOOort + O3 | → | | *ARR1* | 2.62E-16 | | |
| B9-247 | NaOOOort + NO3 | → | | *ARR1* | 3.09E-13 | | |
| B9-248 | NaOOKort + HO | → | | *ARR1* | 1.06E-10 | | |
| B9-249 | NaOOKort + O3 | → | | *ARR1* | 3.74E-18 | | |
| B9-250 | NaOOKort + NO3 | → | | *ARR1* | 8.03E-15 | | |
| B9-251 | PhDOOND + HO | → | | *ARR1* | 3.00E-11 | | |
| B9-252 | PhDOOND + NO3 | → | | *ARR1* | 4.98E-14 | | |
| B9-253 | PhDOOKD + HO | → | | *ARR1* | 2.96E-11 | | |
| B9-254 | PhDOOD1 + HO | → | | *ARR1* | 4.40E-11 | | |
| B9-255 | PhDOOD1 + NO3 | → | | *ARR1* | 5.68E-13 | | |
| B9-256 | PhOOAnhy + HO | → | | *ARR1* | 1.22E-11 | | |
| B9-257 | PhA + HO | → | | *ARR1* | 5.77E-12 | | |
| B9-258 | PhDKND + HO | → | | *ARR1* | 2.52E-11 | | |
| B9-259 | PhDKND + NO3 | → | | *ARR1* | 2.89E-14 | | |
| B9-260 | PhDKHD + HO | → | | *ARR1* | 3.34E-11 | | |
| B9-261 | PhDKHD + NO3 | → | | *ARR1* | 2.89E-14 | | |
| B9-262 | PhOUHEst + HO | → | | *ARR1* | 1.285E-10 | | |
| B9-263 | PhOUAnhy + HO | → | | *ARR2* | 4.96E-11 | | |
| B9-264 | PhOUOEst + HO | → | | *ARR1* | 1.365E-10 | | |
| B9-265 | PhPOUA + HO | → | | *ARR1* | 6.32E-11 | | |
| B9-266 | PhPOUA | → | 3PhOUA + NO2 | *ARR2* | 5.20E+16 | 13850.00 | |
| B9-267 | PhGOUA + HO | → | | *ARR1* | 6.63E-11 | | |
| B9-268 | PhAOUA + HO | → | | *ARR1* | 6.38E-11 | | |
| B9-269 | PhPOUD + HO | → | HO | *ARR1* | 7.02E-11 | | |
| B9-270 | PhPOUD | → | 3PhOUD + NO2 | *ARR2* | 5.20E+16 | 13850.00 | |
| B9-271 | PhGOUD + HO | → | | *ARR1* | 7.33E-11 | | |
| B9-272 | PhAOUD + HO | → | | *ARR1* | 7.07E-11 | | |
| B9-273 | HPhOUA + HO | → | | *ARR1* | 7.33E-11 | | |
| B9-274 | OPhOUA + HO | → | | *ARR1* | 1.125E-10 | | |
| B9-275 | VOPhOUA + HO | → | | *ARR1* | 8.15E-11 | | |
| B9-276 | PhOUP | → | 3PhOU + NO2 | *ARR2* | 5.20E+16 | 13850.00 | |
| B9-277 | PhOUP + HO | → | | *ARR1* | 5.54E-11 | | |
| B9-278 | PhOUG + HO | → | | *ARR1* | 5.85E-11 | | |
| B9-279 | PhOUA + HO | → | | *ARR1* | 5.60E-11 | | |
| B9-280 | NaOKKN + HO | → | | *ARR1* | 2.89E-12 | | |

| | | | | | | |
|---|---|---|---|---|---|---|
| B9-281 | NaOKKH + HO | → | | *ARR1* | 1.76E-11 | |
| B9-282 | NaOKKK + HO | → | | *ARR1* | 3.53E-12 | |
| B9-283 | NaNKON + HO | → | | *ARR1* | 2.65E-12 | |
| B9-284 | NaHKON + HO | → | | *ARR1* | 1.12E-11 | |
| B9-285 | NaOKON + HO | → | | *ARR1* | 1.41E-11 | |
| B9-286 | NaKKON + HO | → | | *ARR1* | 4.76E-12 | |
| B9-287 | PhGND + HO | → | | *ARR1* | 2.85E-11 | |
| B9-288 | PhGND + NO3 | → | | *ARR1* | 1.89E-14 | |
| B9-289 | PhAND + HO | → | | *ARR1* | 2.60E-11 | |
| B9-290 | PhAND + NO3 | → | | *ARR1* | 1.89E-14 | |
| B9-291 | PhPND + HO | → | | *ARR1* | 2.55E-11 | |
| B9-292 | PhPND | → | 3PhND + NO2 | *ARR2* | 5.20E+16 | 13850.00 |
| B9-293 | PhPND + NO3 | → | | *ARR1* | 1.89E-14 | |
| B9-294 | PhNA + HO | → | | *ARR1* | 5.86E-12 | |
| B9-295 | PhNG + HO | → | | *ARR1* | 8.56E-12 | |
| B9-296 | PhNP | → | 3PhN + NO2 | *ARR2* | 5.20E+16 | 13850.00 |
| B9-297 | PhNP + HO | → | | *ARR1* | 5.24E-12 | |
| B9-298 | PhAnhy + HO | → | | *ARR1* | 8.44E-13 | |
| B9-299 | PhEstH + HO | → | 0.55 PhAnhy | *ARR1* | 1.01E-11 | |
| B9-300 | PhEstO + HO | → | 0.28 PhAnhy | *ARR1* | 1.59E-11 | |
| B9-301 | PhGA + HO | → | | *ARR1* | 1.61E-11 | |
| B9-302 | PhPA + HO | → | | *ARR1* | 1.30E-11 | |
| B9-303 | PhAA + HO | → | 0.1 3PhA | *ARR1* | 1.36E-11 | |
| B9-304 | PhPA | → | 3PhA + NO2 | *ARR2* | 5.20E+16 | 13850.00 |
| B9-305 | HPhA + HO | → | 0.23 3PhA | *ARR1* | 1.64E-11 | |
| B9-306 | OPhA + HO | → | 0.1 1PhA | *ARR1* | 3.44E-11 | |
| B9-307 | VOPhA + HO | → | | *ARR1* | 4.93E-12 | |
| B9-308 | PhGD + HO | → | 0.20 3PhD | *ARR1* | 1.64E-11 | |
| B9-309 | PhPD | → | 3PhD + NO2 | *ARR2* | 5.20E+16 | 13850.00 |
| B9-310 | PhPD + HO | → | | *ARR1* | 1.64E-11 | |
| B9-311 | HPhD + HO | → | 0.23 3PhD | *ARR1* | 1.64E-11 | |
| B9-312 | VOPhD + HO | → | | *ARR1* | 9.40E-12 | |
| B9-313 | NaOOO + HO | → | | *ARR1* | 4.955E-10 | |
| B9-314 | NaVOO + HO | → | | *ARR1* | 1.00E-10 | |
| B9-315 | NaHO + HO | → | | *ARR1* | 7.80E-11 | |
| B9-316 | NaOOK + HO | → | | *ARR1* | 7.51E-11 | |
| B9-317 | NaOOK + O3 | → | | *ARR1* | 8.39E-17 | |
| B9-318 | NaOOK + NO3 | → | | *ARR1* | 3.09E-13 | |
| B9-319 | NaOOONBp + HO | → | | *ARR1* | 2.06E-10 | |
| B9-320 | NaOOONBp + NO3 | → | | *ARR1* | 9.08E-13 | |
| B9-321 | NaOOOHBp + HO | → | | *ARR1* | 2.17E-10 | |
| B9-322 | NaOOOHBp + NO3 | → | | *ARR1* | 4.45E-12 | |
| B9-323 | NaOOOOBp + HO | → | | *ARR1* | 2.06E-10 | |
| B9-324 | NaOOOOBp + NO3 | → | | *ARR1* | 9.08E-13 | |

***MO2 (CH3O2.) and MOH (CH3OH) are species from RACM2***

**Table S4: kinetics.**

| kinetic type | formula |
|---|---|
| *ARR1* | $k = x_1$ |
| *ARR1(XX)* | $k = x_1\,[XX]$ |
| *ARR2* | $k = x_1\ e^{\frac{-x_2}{T}}$ |
| *ARR2(XX)* | $k = x_1\ e^{\frac{-x_2}{T}}\ [XX]$ |
| *ARR3* | $k = x_1\ T^{x_2}\ e^{\frac{-x_3}{T}}$ |
| *PHOTO* | $k = x_1$ (value associated to experimental UV lamps see table S5 for atmospheric values depending on zenithal angles) |

**Table S5: atmospheric photolysis rates.**

| reaction ID | reaction | | | atmospheric photolysis rates at sea level for the following zenithal angles: 0, 10, 20, 30, 40, 50, 60, 70, 78, 86, 90. | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| B1-003 | NaV | → | 1Na + NO | 2.1526E-04 | 2.1268E-04 | 2.0491E-04 | 1.9159E-04 | 1.7219E-04 | 1.4589E-04 | 1.1178E-04 | 7.0091E-05 | 3.5657E-05 | 1.0972E-05 | 0.0000E+00 |
| B3-008 | NaOPEN | → | 3PhU + CO + HO2 | 4.7518E-05 | 4.6558E-05 | 4.3706E-05 | 3.9012E-05 | 3.2618E-05 | 2.4837E-05 | 1.6330E-05 | 8.3723E-06 | 3.6409E-06 | 8.8371E-07 | 0.0000E+00 |
| B3-009 | NaOPEN | → | PhDD + 2.0 CO + 2.0 HO2 | 2.9336E-06 | 2.8914E-06 | 2.7643E-06 | 2.5488E-06 | 2.2406E-06 | 1.8363E-06 | 1.3410E-06 | 7.9317E-07 | 3.9615E-07 | 1.2047E-07 | 0.0000E+00 |
| B3-010 | NaOPEN | → | 5PhDCrg + CO | 2.8473E-06 | 2.8063E-06 | 2.6830E-06 | 2.4738E-06 | 2.1747E-06 | 1.7823E-06 | 1.3016E-06 | 7.6984E-07 | 3.8450E-07 | 1.1692E-07 | 0.0000E+00 |
| B3-011 | NaOPEN | → | 4NaOPEN2 + HO2 | 2.8473E-06 | 2.8063E-06 | 2.6830E-06 | 2.4738E-06 | 2.1747E-06 | 1.7823E-06 | 1.3016E-06 | 7.6984E-07 | 3.8450E-07 | 1.1692E-07 | 0.0000E+00 |
| B5.3-008 | ONaOPEN | → | 3OPhU + CO + HO2 | 4.7518E-05 | 4.6558E-05 | 4.3706E-05 | 3.9012E-05 | 3.2618E-05 | 2.4837E-05 | 1.6330E-05 | 8.3723E-06 | 3.6409E-06 | 8.8371E-07 | 0.0000E+00 |
| B5.3-009 | ONaOPEN | → | OPhDD + 2.0 CO + 2.0 HO2 | 2.9336E-06 | 2.8914E-06 | 2.7643E-06 | 2.5488E-06 | 2.2406E-06 | 1.8363E-06 | 1.3410E-06 | 7.9317E-07 | 3.9615E-07 | 1.2047E-07 | 0.0000E+00 |
| B5.3-010 | ONaOPEN | → | 5OPhDCrg + CO | 2.8473E-06 | 2.8063E-06 | 2.6830E-06 | 2.4738E-06 | 2.1747E-06 | 1.7823E-06 | 1.3016E-06 | 7.6984E-07 | 3.8450E-07 | 1.1692E-07 | 0.0000E+00 |
| B5.3-011 | ONaOPEN | → | 4ONaOPEN + HO2 | 2.8473E-06 | 2.8063E-06 | 2.6830E-06 | 2.4738E-06 | 2.1747E-06 | 1.7823E-06 | 1.3016E-06 | 7.6984E-07 | 3.8450E-07 | 1.1692E-07 | 0.0000E+00 |
| B5.6-021 | PhNDKD | → | PhKDD + NO2 + CO + HO2 | 2.4221E-06 | 2.3612E-06 | 2.1827E-06 | 1.8975E-06 | 1.5263E-06 | 1.1023E-06 | 6.7659E-07 | 3.1883E-07 | 1.2888E-07 | 2.9137E-08 | 0.0000E+00 |
| B5.6-022 | PhNDKD | → | PhKDD + CO + NO2 + HO2 | 1.7676E-05 | 1.7243E-05 | 1.5970E-05 | 1.3924E-05 | 1.1243E-05 | 8.1515E-06 | 5.0161E-06 | 2.3590E-06 | 9.4442E-07 | 2.0833E-07 | 0.0000E+00 |
| B5.6-023 | PhNDKD | → | 3PhND + CO + HO2 | 7.6968E-05 | 7.5838E-05 | 7.2455E-05 | 6.6780E-05 | 5.8776E-05 | 4.8426E-05 | 3.5847E-05 | 2.1662E-05 | 1.0736E-05 | 3.1607E-06 | 0.0000E+00 |
| B6-002 | PhDD | → | 0.40 2PhEst + 0.60 3PhD + HO2 | 4.8875E-04 | 4.8275E-04 | 4.6463E-04 | 4.3358E-04 | 3.8835E-04 | 3.2719E-04 | 2.4847E-04 | 1.5397E-04 | 7.8188E-05 | 2.4300E-05 | 0.0000E+00 |
| B6-003 | PhDD | → | 0.40 2PhEst + 0.60 3PhD + HO2 | 4.8875E-04 | 4.8275E-04 | 4.6463E-04 | 4.3358E-04 | 3.8835E-04 | 3.2719E-04 | 2.4847E-04 | 1.5397E-04 | 7.8188E-05 | 2.4300E-05 | 0.0000E+00 |
| B8-011 | GLYOX | → | 2.0 CO | 4.4037E-06 | 4.3088E-06 | 4.0280E-06 | 3.5702E-06 | 2.9552E-06 | 2.2207E-06 | 1.4365E-06 | 7.2308E-07 | 3.1019E-07 | 7.4586E-08 | 0.0000E+00 |
| B8-012 | GLYOX | → | 2.0 CO + 2.0 HO2 | 3.2716E-05 | 3.2197E-05 | 3.0644E-05 | 2.8043E-05 | 2.4392E-05 | 1.9722E-05 | 1.4180E-05 | 8.2364E-06 | 3.9854E-06 | 1.1449E-06 | 0.0000E+00 |
| B8-013 | GLYOX | → | CH2O + CO | 1.8343E-05 | 1.7972E-05 | 1.6870E-05 | 1.5061E-05 | 1.2604E-05 | 9.6214E-06 | 6.3626E-06 | 3.2994E-06 | 1.4538E-06 | 3.6451E-07 | 0.0000E+00 |
| B8-020 | GLYG | → | CHOOH + CO2 | 1.3261E-04 | 1.3095E-04 | 1.2594E-04 | 1.1735E-04 | 1.0485E-04 | 8.7987E-05 | 6.6401E-05 | 4.0830E-05 | 2.0779E-05 | 6.5377E-06 | 0.0000E+00 |
| B8-021 | GLYG | → | CO + CO2 | 1.6681E-05 | 1.6486E-05 | 1.5897E-05 | 1.4884E-05 | 1.3399E-05 | 1.1370E-05 | 8.7149E-06 | 5.4526E-06 | 2.7763E-06 | 8.7201E-07 | 0.0000E+00 |
| B8-023 | GLYA | → | CH2O + CO2 | 1.3261E-04 | 1.3095E-04 | 1.2594E-04 | 1.1735E-04 | 1.0485E-04 | 8.7987E-05 | 6.6401E-05 | 4.0830E-05 | 2.0779E-05 | 6.5377E-06 | 0.0000E+00 |
| B8-024 | GLYA | → | 2.0 CO | 1.6681E-05 | 1.6486E-05 | 1.5897E-05 | 1.4884E-05 | 1.3399E-05 | 1.1370E-05 | 8.7149E-06 | 5.4526E-06 | 2.7763E-06 | 8.7201E-07 | 0.0000E+00 |
| B8-028 | CH2O | → | 2.0 HO2 + CO | 2.8961E-05 | 2.8360E-05 | 2.6576E-05 | 2.3652E-05 | 1.9690E-05 | 1.4905E-05 | 9.7259E-06 | 4.9364E-06 | 2.1192E-06 | 4.9897E-07 | 0.0000E+00 |
| B8-029 | CH2O | → | CO | 3.9749E-05 | 3.9115E-05 | 3.7212E-05 | 3.4012E-05 | 2.9497E-05 | 2.3696E-05 | 1.6820E-05 | 9.5893E-06 | 4.6494E-06 | 1.3289E-06 | 0.0000E+00 |

# Part 2: Modeling data

**Table S6: Final concentrations of simulated secondary species (in µg/m3).**

| m/z | species | Gas | Part. |
|---|---|---|---|
| 31 | CH2O | 0.018 | 0 |
| 47 | CHOOH | 0 | 0 |
| 59 | GLYOX | 7.398 | 0 |
| 75 | GLYA | 0.002 | 0 |
| 91 | GLYG | 0 | 0 |
| 95 | OPh | 0 | 0 |
| 107 | PhD | 0.144 | 0 |
| 111 | HPh | 0 | 0 |
| 123 | PhA | 0.013 | 0 |
| 123 | OPhD | 0.007 | 0 |
| 129 | NAPH | 20.078 | 0 |
| 135 | PhDD | 9.804 | 0.004 |
| 135 | PhKD | 0.016 | 0 |
| 137 | PhOD | 0 | 0 |
| 139 | HPhD | 0 | 0 |
| 139 | OPhA | 0 | 0 |
| 140 | VOPh | 0.027 | 0 |
| 145 | NaO | 1.397 | 0 |
| 149 | PhAnhy | 1.15 | 0.163 |
| 149 | PhUA | 0 | 0 |
| 149 | PhDCD | 0.005 | 0 |
| 151 | PhEstO | 0 | 0 |
| 151 | OPhDD | 0.069 | 0.008 |
| 151 | PhKA | 0 | 0 |
| 151 | PhAD | 0.422 | 0.023 |
| 153 | PhOA | 0 | 0 |
| 153 | PhHD | 0 | 0 |
| 155 | HPhA | 0 | 0 |
| 159 | NaKK | 0.32 | 0 |
| 159 | NaQuin | 0.697 | 0 |
| 161 | ONaO | 0.116 | 0.009 |
| 161 | NaH | 0 | 0 |
| 161 | NaOPEN | 2.859 | 0.041 |
| 161 | NaOKpar | 0.944 | 0.003 |
| 161 | NaOKort | 0.595 | 0.002 |
| 161 | NaOO | 0.084 | 0.007 |
| 163 | NaOOpar | 0 | 0 |
| 163 | NaOOort | 0 | 0 |
| 163 | PhKDD | 0.139 | 0.001 |
| 165 | OPhDCD | 0 | 0 |
| 165 | PhDCA | 0.002 | 0 |
| 165 | PhOUA | 0 | 0 |
| 165 | PhUG | 0 | 0 |
| 165 | PhDOD | 0 | 0 |
| 165 | PhEpoxA | 0 | 0 |
| 165 | OPhUA | 0 | 0 |
| 167 | OPhAD | 0.001 | 0.002 |
| 167 | PhEstH | 0 | 0 |
| 167 | PhGD | 0 | 0 |
| 167 | PhKG | 0 | 0 |
| 167 | OPhKA | 0 | 0 |
| 167 | PhAA | 0.006 | 0.015 |
| 168 | VOPhD | 0.782 | 0.088 |
| 169 | PhOG | 0 | 0 |
| 169 | OPhOA | 0 | 0 |
| 174 | NaV | 2.935 | 0.001 |
| 175 | ONaQuin | 0.005 | 0 |
| 175 | NaKKEpox | 2.886 | 0.002 |
| 175 | PhUAnhy | 0.194 | 0.207 |
| 177 | NaOPENEpox | 0.838 | 0.001 |
| 177 | NaOOO | 0.015 | 0.031 |
| 177 | PhKAnhy | 0.015 | 0.024 |
| 177 | NaOPENOL | 0.167 | 0.229 |
| 177 | NaHO | 0 | 0 |
| 177 | NaOOK | 0.064 | 0.024 |
| 177 | ONaOPEN | 0.05 | 0.11 |
| 177 | NaOKEpox | 0.024 | 0 |
| 177 | ONaOKort | 0 | 0 |
| 177 | NaOOKort | 0 | 0 |
| 177 | ONaOKpar | 0.013 | 0.009 |
| 177 | PhUOEst1 | 0 | 0 |
| 177 | PhAUD1 | 0 | 0 |
| 177 | PhUOEst2 | 0 | 0 |
| 177 | PhAUD2 | 0 | 0 |
| 179 | PhDKA | 0.004 | 0.005 |
| 179 | ONaOOort | 0 | 0 |
| 179 | NaOOOort | 0 | 0 |
| 179 | ONaOOpar | 0 | 0 |
| 179 | NaOHpar | 0 | 0 |
| 179 | PhAKD | 0.007 | 0.011 |
| 179 | NaOHort | 0 | 0 |
| 179 | NaOOEpox | 0 | 0 |
| 181 | OPhDCA | 0 | 0 |
| 181 | PhDOOD1 | 0.019 | 0 |

| m/z | species | Gas | Part. |
|---|---|---|---|
| 181 | PhOUG | 0 | 0 |
| 181 | HPhUA | 0 | 0 |
| 181 | PhDHD | 0 | 0 |
| 181 | PhKOA | 0 | 0 |
| 181 | PhEpoxG | 0 | 0 |
| 181 | PhAOD | 0 | 0 |
| 181 | OOPhUA | 0 | 0 |
| 181 | OPhOUA | 0 | 0 |
| 181 | OPhEpoxA | 0 | 0 |
| 182 | PhND | 0.002 | 0 |
| 183 | PhGA | 0 | 0 |
| 183 | HPhKA | 0 | 0 |
| 184 | VOPhA | 0.152 | 0.388 |
| 185 | HPhOA | 0 | 0 |
| 190 | NaVO | 0.503 | 0.046 |
| 191 | NaOKKK | 0 | 0 |
| 191 | PhKDKD | 0.039 | 0.006 |
| 191 | PhDKKD | 0.207 | 0.033 |
| 191 | PhOUAnhy | 0.009 | 0.031 |
| 191 | PhEpoxAnhy | 0.074 | 0.055 |
| 191 | OPhUAnhy | 0.003 | 0.012 |
| 193 | OPhDEpoxD | 0.005 | 0.001 |
| 193 | PhOUOEst | 0 | 0 |
| 193 | PhGUD1 | 0 | 0 |
| 193 | PhGUD2 | 0 | 0 |
| 193 | PhEpoxOEst | 0 | 0 |
| 193 | PhODKD | 0.258 | 0.439 |
| 193 | PhAOUD | 0 | 0 |
| 193 | PhUHEst1 | 0 | 0 |
| 193 | PhUHEst2 | 0 | 0 |
| 193 | PhAEpoxD | 0.048 | 0.047 |
| 193 | PhDKOD | 0.507 | 0.767 |
| 193 | NaOOKK | 0 | 0 |
| 193 | PhAUA | 0.001 | 0.002 |
| 195 | PhOOAnhy | 0.002 | 0.005 |
| 195 | ONaOHort | 0 | 0 |
| 195 | NaOOHort | 0 | 0 |
| 195 | ONaOHpar | 0 | 0 |
| 195 | NaOHEpox | 0 | 0 |
| 195 | PhDOOD | 0 | 0 |
| 195 | NaOOOK | 0 | 0 |
| 195 | OPhKKA | 0 | 0 |
| 197 | HPhOUA | 0 | 0 |
| 197 | OHPhUA | 0 | 0 |
| 197 | PhKOG | 0 | 0 |
| 197 | PhAHD | 0 | 0 |
| 197 | HPhEpoxA | 0 | 0 |
| 197 | OPhKOA | 0 | 0 |
| 198 | PhNA | 0 | 0 |
| 205 | PhKKAnhy | 0.024 | 0.049 |
| 206 | NaVOO | 0.014 | 0.037 |
| 207 | PhOKAnhy | 0.02 | 0.064 |
| 207 | PhKOAnhy | 0.032 | 0.098 |
| 208 | NaONpar | 0.111 | 0.012 |
| 208 | NaONort | 0.478 | 0.05 |
| 209 | PhDOOKD | 0 | 0 |
| 209 | PhOUHEst | 0 | 0 |
| 209 | PhGOUD | 0 | 0 |
| 209 | NaOKKH | 0 | 0 |
| 209 | OPhODKD | 0.209 | 0.6 |
| 209 | PhOKOEst | 0 | 0 |
| 209 | PhKOOEst | 0 | 0 |
| 209 | PhEpoxHEst | 0 | 0 |
| 209 | ONaOOKK | 0 | 0 |
| 209 | PhDKHD | 0 | 0 |
| 209 | OPhDKOD | 0 | 0 |
| 209 | PhAOKD | 0 | 0 |
| 209 | PhGUA1 | 0 | 0 |
| 209 | PhGUA2 | 0 | 0 |
| 209 | PhGEpoxD | 0 | 0 |
| 209 | PhAOUA | 0 | 0 |
| 209 | OPhAUA | 0 | 0 |
| 209 | PhAKOD | 0 | 0 |
| 209 | PhAEpoxA | 0 | 0.001 |
| 210 | PhUP | 0.137 | 0 |
| 210 | VOPhUA | 0.018 | 0.053 |
| 210 | PhDND | 0.002 | 0 |
| 211 | PhDOOOD | 0 | 0 |
| 211 | HPhKKA | 0 | 0 |
| 211 | ONaOOOK | 0 | 0 |
| 211 | OPhDOOD | 0 | 0 |
| 211 | PhDHOD | 0.001 | 0.002 |
| 211 | NaHOOK | 0 | 0.001 |
| 212 | PhPD | 4.163 | 0.006 |
| 212 | VOPhKA | 0.004 | 0.008 |
| 212 | PhKP | 0.005 | 0 |
| 213 | PhAOOA | 0 | 0 |
| 213 | HPhKOA | 0 | 0 |
| 214 | PhNG | 0 | 0 |
| 214 | VOPhOA | 0.001 | 0.021 |
| 214 | PhOP | 0.054 | 0.001 |
| 223 | PhKAKA | 0 | 0 |
| 224 | ONaONpar | 0.001 | 0.002 |
| 224 | ONaONort | 0.003 | 0.006 |

| m/z | species | Gas | Part. |
|---|---|---|---|
| **224** | **NaONEpox** | 0.309 | 0.029 |
| **224** | **NaOONort** | 0.049 | 0.113 |
| **225** | **PhGOUA** | 0 | 0 |
| **225** | **PhOKHEst** | 0 | 0 |
| **225** | **PhGOKD** | 0 | 0 |
| **225** | **PhKOHEst** | 0 | 0 |
| **225** | **NaOKBp** | 0 | 0 |
| **225** | **PhAOKA** | 0 | 0.001 |
| **225** | **PhAKOA** | 0 | 0.001 |
| **225** | **PhGKOD** | 0 | 0 |
| **225** | **PhAEpoxG** | 0 | 0 |
| **226** | **VOPhOUA** | 0 | 0.016 |
| **226** | **PhOUP** | 0.004 | 0.001 |
| **226** | **VOOPhUA** | 0 | 0.006 |
| **226** | **PhEpoxP** | 0.032 | 0 |
| **226** | **VOPhEpoxA** | 0.008 | 0.02 |
| **226** | **PhAND** | 0.001 | 0.002 |
| **227** | **PhDOOHD** | 0 | 0 |
| **227** | **ONaHOOK** | 0 | 0 |
| **227** | **NaOOBp** | 0 | 0 |
| **227** | **OPhDHOD** | 0 | 0 |
| **228** | **PhPA** | 0.942 | 0.774 |
| **238** | **NaOKKN** | 0.018 | 0.034 |
| **238** | **NaKKON** | 0 | 0 |
| **238** | **PhNDKD** | 0 | 0 |
| **238** | **PhPUD1** | 0.324 | 0.029 |
| **238** | **PhPUD2** | 0.247 | 0.015 |
| **238** | **PhDKND** | 0.006 | 0.008 |
| **240** | **NaOKON** | 0 | 0 |
| **240** | **VOPhKKA** | 0.001 | 0.012 |
| **240** | **PhDNOD** | 0.431 | 1.235 |
| **240** | **NaNOOK** | 0.16 | 0.431 |
| **241** | **PhGOKA** | 0 | 0 |
| **241** | **PhGKOA** | 0 | 0 |
| **241** | **ONaOKBp** | 0 | 0 |
| **241** | **NaOOKBp** | 0.687 | 0.029 |
| **242** | **VOPhKOA** | 0.001 | 0.039 |
| **242** | **PhKOP** | 0.011 | 0.006 |
| **242** | **PhGND** | 0 | 0 |
| **243** | **NaOHBp** | 0 | 0 |
| **243** | **ONaOOBp** | 0 | 0 |
| **243** | **NaOOOBp** | 0 | 0 |
| **254** | **PhPOUD** | 0.015 | 0.04 |
| **254** | **PhPUA1** | 0.096 | 0.233 |
| **254** | **PhPUA2** | 0.069 | 0.168 |
| **254** | **PhPEpoxD** | 0.174 | 0.005 |
| **256** | **NaHKON** | 0 | 0 |

| m/z | species | Gas | Part. |
|---|---|---|---|
| **256** | **PhDOOND** | 0.002 | 0.007 |
| **256** | **OPhDNOD** | 0.005 | 0.016 |
| **256** | **ONaNOOK** | 0.001 | 0.003 |
| **259** | **PhNP** | 0 | 0 |
| **259** | **ONaOHBp** | 0 | 0 |
| **259** | **NaOOHBp** | 0 | 0 |
| **259** | **NaOOOOBp** | 0 | 0 |
| **270** | **PhPOUA** | 0.016 | 0.063 |
| **270** | **PhPOKD** | 0.033 | 0.087 |
| **270** | **PhPKOD** | 0.053 | 0.133 |
| **270** | **PhAEpoxP** | 0.059 | 0.126 |
| **272** | **NaONBp** | 0.122 | 0.002 |
| **275** | **NaOOOHBp** | 0 | 0 |
| **285** | **NaNKON** | 0 | 0 |
| **286** | **PhPOKA** | 0.016 | 0.153 |
| **286** | **PhPKOA** | 0.021 | 0.248 |
| **287** | **PhPND** | 0 | 0 |
| **288** | **ONaONBp** | 0.001 | 0.001 |
| **288** | **NaOONBp** | 0.012 | 0.014 |
| **304** | **NaOOONBp** | 0 | 0 |