

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)	ΔH _{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	c1HcHcHcHc1(OOH)	c1ccccc1(OO)	0.530E-01	66.0
HPhA	154.	7	6	4	0	CO(OH)c1cHcHcHc1(OOH)	C(=O)(O)c1ccccc1(OO)	0.993E-06	115.6
HPhD	138.	7	6	3	0	CHOc1cHcHcHc1(OOH)	C(=O)c1ccccc1(OO)	0.952E-03	82.9
HPhKA	182.	8	6	5	0	c1(OOH)cHcHcHc1COCO(OH)	c1(OO)cccc1C(=O)C(=O)(O)	0.313E-07	130.9
HPhKKA	210.	9	6	6	0	c1(OOH)cHcHcHc1COCOCO(OH)	c1(OO)cccc1C(=O)C(=O)C(=O)(O)	0.383E-09	151.5
HPhKOA	212.	9	8	6	0	c1(OOH)cHcHcHc1COCH(OH)CO(OH)	c1(OO)cccc1C(=O)C(O)C(=O)(O)	0.184E-10	167.3
HPhOA	184.	8	8	5	0	c1(OOH)cHcHcHc1CH(OH)CO(OH)	c1(OO)cccc1C(O)C(=O)(O)	0.101E-08	148.8
HPhOUA	196.	9	8	5	0	c1(OOH)cHcHcHc1CdH=CdHCO(OH)	c1(OO)cccc1C(O)=CC(=O)(O)	0.791E-10	160.7
HPhUA	180.	9	8	4	0	c1(OOH)cHcHcHc1CdH=CdHCO(OH)	c1(OO)cccc1C=CC(=O)(O)	0.131E-07	135.2
NaH	160.	10	8	2	0	c12cHcHcHc1cHcHc2(OOH)	c12ccccc1cccc2(OO)	0.842E-07	122.8
NaHKON	255.	10	9	7	1	c12cHcHcHc1CH(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	c12cHcHcHc1cHcHc(OOH)c2(OH)	c12ccccc1ccc(OO)c2(O)	0.365E-09	149.1
NaHOOK	210.	10	10	5	0	c12cHcHcHc1COCH(OH)CH(OOH)C2H(OH)	c12ccccc1C(=O)C(O)C(OO)C2(O)	0.742E-09	149.5
NaKK	158.	10	6	2	0	c12cHcHcHc1CdH=CdHCO2O	c12ccccc1C=CC(=O)C2=O	0.394E-02	72.9
NaKKON	237.	10	7	6	1	c12cHcHcHc1CH(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	c12cHcHcHc1CH(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	c12cHcHcHc1COCH(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	c12cHcHcHc1cHcHc2(OH)	c12ccccc1cccc2(O)	0.600E-05	102.0
NaOHBP	242.	10	10	7	0	c12cHcHcHc1CH(OOH)C3HCH(OH)C2H-O--O3-	c12ccccc1C(OO)C3C(O)C2O03	0.231E-04	102.2

Name	MW (g mol ⁻¹)	nbC	nbH	nbO	nbN	Chem code (GECKO-A)	Smile code	P ^{sat} (torr)	ΔH ^{vap} (kJ)
NaOHort	178.	10	10	3	0	c12cHcHcHcHc1CdH=CdHCH(OOH)C2H(OH)	c12cccc1C=CC(OO)C2(O)	0.221E-05	111.0
NaOHpar	178.	10	10	3	0	c12cHcHcHcHc1CH(OOH)CdH=CdHC2H(OH)	c12cccc1C(OO)C=CC2(O)	0.221E-05	111.0
NaOKBp	224.	10	8	6	0	c12cHcHcHcHc1COC3HCH(OH)C2H-O--O3-	c12cccc1C(=O)C3C(O)C2O03	0.296E-02	78.2
NaOKKH	208.	10	8	5	0	c12cHcHcHcHc1CH(OH)CH(OOH)COC2O	c12cccc1C(O)C(OO)C(=O)C2=O	0.974E-08	135.9
NaOKKK	190.	10	6	4	0	c12cHcHcHcHc1CH(OH)COCOC2O	c12cccc1C(O)C(=O)C(=O)C2=O	0.188E-05	110.1
NaOKKN	237.	10	7	6	1	c12cHcHcHcHc1CH(OH)CH(ONO2)COC2O	c12cccc1C(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	c12cccc1C(ON(=O)=O)C(O)C(O)C2=O	0.129E-07	135.7
NaOKort	160.	10	8	2	0	c12cHcHcHcHc1CdH=CdHCH(OH)C2O	c12cccc1C=CC(O)C2=O	0.607E-03	83.4
NaOKpar	160.	10	8	2	0	c12cHcHcHcHc1COCdH=CdHC2H(OH)	c12cccc1C(=O)C=CC2(O)	0.448E-03	84.5
NaONBp	271.	10	9	8	1	c12cHcHcHcHc1CH(ONO2)C3HCH(OH)C2H-O--O3-	c12cccc1C(ON(=O)=O)C3C(O)C2O03	0.122E-03	94.3
NaONort	207.	10	9	4	1	c12cHcHcHcHc1CdH=CdHCH(ONO2)C2H(OH)	c12cccc1C=CC(ON(=O)=O)C2(O)	0.229E-04	100.3
NaONpar	207.	10	9	4	1	c12cHcHcHcHc1CH(ONO2)CdH=CdHC2H(OH)	c12cccc1C(ON(=O)=O)C=CC2(O)	0.229E-04	100.3
NaOO	160.	10	8	2	0	c12cHcHcHcHc1cHcHc(OH)c2(OH)	c12cccc1ccc(O)c2(O)	0.398E-07	125.8
NaOOBp	226.	10	10	6	0	c12cHcHcHcHc1CH(OH)C3HCH(OH)C2H-O--O3-	c12cccc1C(O)C3C(O)C2O03	0.317E-03	90.9
NaOOHBp	258.	10	10	8	0	c12cHcHcHcHc1CH(OOH)C3HCH(OH)C2(OH)-O--O3-	c12cccc1C(OO)C3C(O)C2(O)O03	0.313E-06	123.5
NaOOHort	194.	10	10	4	0	c12cHcHcHcHc1CH(OH)CH(OOH)CdH=Cd2(OH)	c12cccc1C(O)C(OO)C=C2(O)	0.217E-07	134.2
NaOOK	176.	10	8	3	0	c12cHcHcHcHc1Cd(OH)=CdHCH(OH)C2O	c12cccc1C(O)=CC(O)C2=O	0.705E-05	106.0
NaOOKBp	240.	10	8	7	0	c12cHcHcHcHc1COC3HCH(OH)C2(OH)-O--O3-	c12cccc1C(=O)C3C(O)C2(O)O03	0.533E-04	98.4
NaOOKK	192.	10	8	4	0	c12cHcHcHcHc1COCH(OH)COC2H(OH)	c12cccc1C(=O)C(O)C(=O)C2(O)	0.191E-06	122.3
NaOOKort	176.	10	8	3	0	c12cHcHcHcHc1CH(OH)COCdH=Cd2(OH)	c12cccc1C(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-	c12cccc1C(ON(=O)=O)C3C(O)C2(O)O03	0.193E-05	114.4
NaOONort	223.	10	9	5	1	c12cHcHcHcHc1CH(OH)CH(ONO2)CdH=Cd2(OH)	c12cccc1C(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)	c12cccc1cc(O)c(O)c2(O)	0.183E-09	152.4
NaOOOBp	242.	10	10	7	0	c12cHcHcHcHc1CH(OH)C3HCH(OH)C2(OH)-O--O3-	c12cccc1C(O)C3C(O)C2(O)O03	0.564E-05	110.9
NaOOOHBp	274.	10	10	9	0	c12cHcHcHcHc1C(OH)(OOH)C3HCH(OH)C2(OH)-O--O3-	c12cccc1C(O)(OO)C3C(O)C2(O)O03	0.346E-08	145.9
NaOOOK	194.	10	10	4	0	c12cHcHcHcHc1COCH(OH)CH(OH)C2H(OH)	c12cccc1C(=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-	c12cccc1C(O)(ON(=O)=O)C3C(O)C2(O)O03	0.284E-07	135.6
NaOOOObp	258.	10	10	8	0	c12cHcHcHcHc1C(OH)(OH)C3HCH(OH)C2(OH)-O--O3-	c12cccc1C(O)(O)C3C(O)C2(O)O03	0.316E-04	103.7
NaOOOort	178.	10	10	3	0	c12cHcHcHcHc1CH(OH)CH(OH)CdH=Cd2(OH)	c12cccc1C(O)C(O)C=C2(O)	0.493E-06	120.3

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NaOOort	162.	10	10	2	0	c12cHcHcHcHc1CdH=CdHCH(OH)C2H(OH)	c12cccc1C=CC(O)C2(O)	0.371E-04	98.6
NaOOpAr	162.	10	10	2	0	c12cHcHcHcHc1CH(OH)CdH=CdHC2H(OH)	c12cccc1C(O)C=CC2(O)	0.371E-04	98.6
NaOPEN	160.	10	8	2	0	CHOc1cHcHcHcHc1CdH=CdHCHO	C(=O)c1cccc1C=CC=O	0.271E-03	86.5
NaOPENOL	176.	10	8	3	0	CHOc1cHcHcHcHc1Cd(OH)=CdHCHO	C(=O)c1cccc1C(O)=CC=O	0.461E-05	107.0
NAPH	128.	10	8	0	0	c12cHcHcHcHc1cHcHcHc2H	c12cccc1cccc2	0.503E-03	81.0
NaQuin	158.	10	6	2	0	c12cHcHcHcHc1COCdH=CdHC2O	c12cccc1C(=O)C=CC2=O	0.566E-02	70.9
NaV	173.	10	7	2	1	c12cHcHcHcHc1cHcHcHc2(NO2)	c12cccc1cccc2(N(=O)=O)	0.415E-05	102.8
NaVO	189.	10	7	3	1	c12cHcHcHcHc1cHcHc(OH)c2(NO2)	c12cccc1ccc(O)c2(N(=O)=O)	0.348E-07	126.1
NaVOO	205.	10	7	4	1	c12cHcHcHcHc1cHc(OH)c(NO2)c2(OH)	c12cccc1cc(O)c(N(=O)=O)c2(O)	0.176E-09	152.1
OHPPhUA	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)C2O03	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)C2O03	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)C2O03	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)C2O03	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)	ΔH ^{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	c1HcHcHcHc1(OH)	c1cccc1(O)	0.153E+01	50.9
OPhA	138.	7	6	3	0	CO(OH)c1cHcHcHc1(OH)	C(=O)(O)c1cccc1(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)cHcHcHc1COCO(OH)	c1(O)cccc1C(=O)C(=O)(O)	0.267E-05	109.8
OPhKKA	194.	9	6	5	0	c1(OH)cHcHcHc1COCOCO(OH)	c1(O)cccc1C(=O)C(=O)C(=O)(O)	0.420E-07	128.8
OPhKOA	196.	9	8	5	0	c1(OH)cHcHcHc1COCH(OH)CO(OH)	c1(O)cccc1C(=O)C(O)C(=O)(O)	0.266E-08	143.2
OPhOA	168.	8	8	4	0	c1(OH)cHcHcHc1CH(OH)CO(OH)	c1(O)cccc1C(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)cHcHcHc1Cd(OH)=CdHCO(OH)	c1(O)cccc1C(O)=CC(=O)(O)	0.109E-07	137.1
OPhUA	164.	9	8	3	0	c1(OH)cHcHcHc1CdH=CdHCO(OH)	c1(O)cccc1C=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	c1HcHcHcHc1CO(OH)	c1cccc1C(=O)(O)	0.892E-02	74.1
PhAA	166.	8	6	4	0	CO(OH)c1cHcHcHc1CO(OH)	C(=O)(O)c1cccc1C(=O)(O)	0.471E-06	117.6
PhAD	150.	8	6	3	0	CHOc1cHcHcHc1CO(OH)	C(=O)c1cccc1C(=O)(O)	0.117E-03	92.3
PhAKD	178.	9	6	4	0	CHOCOc1cHcHcHc1CO(OH)	O=CC(=O)c1cccc1C(=O)(O)	0.397E-05	107.3
PhAKOA	224.	10	8	6	0	CO(OH)c1cHcHcHc1COCH(OH)CO(OH)	C(=O)(O)c1cccc1C(=O)C(O)C(=O)(O)	0.145E-11	179.5
PhAKOD	208.	10	8	5	0	CO(OH)c1cHcHcHc1COCH(OH)CHO	C(=O)(O)c1cccc1C(=O)C(O)C=O	0.414E-08	140.5
PhAND	225.	9	7	6	1	CO(OH)c1cHcHcHc1CH(ONO2)CHO	C(=O)(O)c1cccc1C(ON(=O)=O)C=O	0.119E-06	124.7
PhAnhy	148.	8	4	3	0	c12cHcHcHc1CO-O-C2O	c12cccc1C(=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)	ΔH ^{vap} (kJ)
PhAOCA	210.	10	10	5	0	CO(OH)c1cHcHcHcHc1CH(OH)CH2CO(OH)	C(=O)(O)c1cccc1C(O)CC(=O)(O)	0.294E-10	165.3
PhAOCD	194.	10	10	4	0	CO(OH)c1cHcHcHcHc1CH(OH)CH2CHO	C(=O)(O)c1cccc1C(O)CC=O	0.426E-07	130.0
PhAOCG	226.	10	10	6	0	CO(OH)c1cHcHcHcHc1CH(OH)CH2CO(OOH)	C(=O)(O)c1cccc1C(O)CC(=O)(OO)	0.249E-09	155.2
PhAOCP	271.	10	9	8	1	CO(OH)c1cHcHcHcHc1CH(OH)CH2CO(OON02)	C(=O)(O)c1cccc1C(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)c1cccc1C(O)C=O	0.136E-06	124.8
PhAOH	198.	9	10	5	0	CO(OH)c1cHcHcHcHc1CH(OH)CH2(OOH)	C(=O)(O)c1cccc1C(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)c1cccc1C(=O)C(=O)(O)	0.145E-11	179.5
PhAOKD	208.	10	8	5	0	CHOC0c1cHcHcHcHc1CH(OH)CO(OH)	O=CC(=O)c1cccc1C(O)C(=O)(O)	0.414E-08	140.5
PhAON	227.	9	9	6	1	CO(OH)c1cHcHcHcHc1CH(OH)CH2(ON02)	C(=O)(O)c1cccc1C(O)C(ON(=O)=O)	0.430E-08	141.5
PhA00	182.	9	10	4	0	CO(OH)c1cHcHcHcHc1CH(OH)CH2(OH)	C(=O)(O)c1cccc1C(O)C(O)	0.402E-08	142.1
PhA00A	212.	9	8	6	0	CO(OH)c1cHcHcHcHc1C(OH)(OH)CO(OH)	C(=O)(O)c1cccc1C(O)(O)C(=O)(O)	0.131E-08	148.0
PhA0UA	208.	10	8	5	0	CO(OH)c1cHcHcHcHc1Cd(OH)=CdHCO(OH)	C(=O)(O)c1cccc1C(O)=CC(=O)(O)	0.758E-11	171.7
PhA0UD	192.	10	8	4	0	CO(OH)c1cHcHcHcHc1Cd(OH)=CdHCHO	C(=O)(O)c1cccc1C(O)=CC=O	0.131E-07	135.5
PhAUA	192.	10	8	4	0	CO(OH)c1cHcHcHcHc1CdH=CdHCO(OH)	C(=O)(O)c1cccc1C=CC(=O)(O)	0.566E-08	138.1
PhAUD1	176.	10	8	3	0	CO(OH)c1cHcHcHcHc1CdH=CdHCHO	C(=O)(O)c1cccc1C=CC=O	0.189E-05	110.8
PhAUD2	176.	10	8	3	0	CHOc1cHcHcHcHc1CdH=CdHCO(OH)	C(=O)c1cccc1C=CC(=O)(O)	0.227E-05	109.8
PhD	106.	7	6	1	0	c1HcHcHcHc1CHO	c1cccc1C=O	0.144E+01	49.7
PhDCA	164.	9	8	3	0	CHOc1cHcHcHcHc1CH2CO(OH)	C(=O)c1cccc1CC(=O)(O)	0.501E-04	96.3
PhDCD	148.	9	8	2	0	CHOc1cHcHcHcHc1CH2CHO	C(=O)c1cccc1CC=O	0.386E-02	75.3
PhDD	134.	8	6	2	0	CHOc1cHcHcHcHc1CHO	C(=O)c1cccc1C=O	0.842E-02	71.3
PhDHOD	210.	10	10	5	0	CHOc1cHcHcHcHc1CH(OOH)CH(OH)CHO	C(=O)c1cccc1C(OO)C(O)C=O	0.854E-08	137.1
PhDKA	178.	9	6	4	0	CHOc1cHcHcHcHc1COCO(OH)	C(=O)c1cccc1C(=O)C(=O)(O)	0.473E-05	106.2
PhDKHD	208.	10	8	5	0	CHOc1cHcHcHcHc1COCH(OOH)CHO	C(=O)c1cccc1C(=O)C(OO)C=O	0.288E-06	118.9
PhDKKD	190.	10	6	4	0	CHOc1cHcHcHcHc1COCOCHO	C(=O)c1cccc1C(=O)C(=O)C=O	0.429E-04	94.4
PhDKND	237.	10	7	6	1	CHOc1cHcHcHcHc1COCH(ON02)CHO	C(=O)c1cccc1C(=O)C(ON(=O)=O)C=O	0.272E-05	108.0
PhDKOD	192.	10	8	4	0	CHOc1cHcHcHcHc1COCH(OH)CHO	C(=O)c1cccc1C(=O)C(O)C=O	0.438E-05	106.6
PhDNOD	239.	10	9	6	1	CHOc1cHcHcHcHc1CH(ON02)CH(OH)CHO	C(=O)c1cccc1C(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)c1cccc1C(O)C(O)C=O	0.166E-06	123.6
PhDOOD1	180.	9	8	4	0	CHOc1cHcHcHcHc1C(OH)(OH)CHO	C(=O)c1cccc1C(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)	ΔH ^{vap} (kJ)
PhDOOHD	226.	10	10	6	0	CHOc1cHcHcHcHc1C(OH)(OH)CH(OOH)CHO	C(=O)c1cccc1C(O)(O)C(OO)C=O	0.731E-07	127.5
PhDOOKD	208.	10	8	5	0	CHOc1cHcHcHcHc1C(OH)(OH)COCHO	C(=O)c1cccc1C(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)c1cccc1C(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)c1cccc1C(O)(O)C(O)C=O	0.128E-05	114.7
PhEstH	166.	8	6	4	0	c12cHcHcHcHc1CO-O-C2H(OOH)	c12cccc1C(=O)OC2(OO)	0.702E-05	102.4
PhEstO	150.	8	6	3	0	c12cHcHcHcHc1CO-O-C2H(OH)	c12cccc1C(=O)OC2(O)	0.988E-04	90.4
PhGA	182.	8	6	5	0	CO(OH)c1cHcHcHcHc1CO(OOH)	C(=O)(O)c1cccc1C(=O)(OO)	0.255E-05	109.9
PhGD	166.	8	6	4	0	CHOc1cHcHcHcHc1CO(OOH)	C(=O)c1cccc1C(=O)(OO)	0.492E-03	85.7
PhGKOA	240.	10	8	7	0	CO(OH)c1cHcHcHcHc1COCH(OH)CO(OOH)	C(=O)(O)c1cccc1C(=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)c1cccc1C(=O)C(O)C=O	0.262E-07	131.8
PhGND	241.	9	7	7	1	CO(OOH)c1cHcHcHcHc1CH(ONO2)CHO	C(=O)(OO)c1cccc1C(ON(=O)=O)C=O	0.577E-06	117.2
PhGOCD	210.	10	10	5	0	CO(OOH)c1cHcHcHcHc1CH(OH)CH2CHO	C(=O)(OO)c1cccc1C(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)c1cccc1C(=O)C(=O)(OO)	0.137E-10	168.7
PhGOKD	224.	10	8	6	0	CHOCOc1cHcHcHcHc1CH(OH)CO(OOH)	O=CC(=O)c1cccc1C(O)C(=O)(OO)	0.262E-07	131.8
PhGOUA	224.	10	8	6	0	CO(OH)c1cHcHcHcHc1Cd(OH)=CdHCO(OOH)	C(=O)(O)c1cccc1C(O)=CC(=O)(OO)	0.703E-10	161.1
PhGOUD	208.	10	8	5	0	CO(OOH)c1cHcHcHcHc1Cd(OH)=CdHCHO	C(=O)(OO)c1cccc1C(O)=CC=O	0.846E-07	126.8
PhGUA1	208.	10	8	5	0	CO(OH)c1cHcHcHcHc1CdH=CdHCO(OOH)	C(=O)(O)c1cccc1C=CC(=O)(OO)	0.360E-07	129.4
PhGUA2	208.	10	8	5	0	CO(OOH)c1cHcHcHcHc1CdH=CdHCO(OH)	C(=O)(OO)c1cccc1C=CC(=O)(O)	0.360E-07	129.4
PhGUD1	192.	10	8	4	0	CO(OOH)c1cHcHcHcHc1CdH=CdHCHO	C(=O)(OO)c1cccc1C=CC=O	0.943E-05	103.4
PhGUD2	192.	10	8	4	0	CHOc1cHcHcHcHc1CdH=CdHCO(OOH)	C(=O)c1cccc1C=CC(=O)(OO)	0.112E-04	102.3
PhKA	150.	8	6	3	0	c1HcHcHcHcHc1COCO(OH)	c1cccc1C(=O)C(=O)(O)	0.404E-03	86.4
PhKAKA	222.	10	6	6	0	CO(OH)COc1cHcHcHcHc1COCO(OH)	C(=O)(O)C(=O)c1cccc1C(=O)C(=O)(O)	0.631E-10	160.0
PhKANhy	176.	9	4	4	0	c12cHcHcHcHc1COCO-O-C2O	c12cccc1C(=O)C(=O)OC2=O	0.625E-06	112.4
PhKD	134.	8	6	2	0	c1HcHcHcHcHc1COCHO	c1cccc1C(=O)C=O	0.107E+00	60.7
PhKDD	162.	9	6	3	0	CHOCOc1cHcHcHcHc1CHO	O=CC(=O)c1cccc1C=O	0.128E-02	79.2
PhKDKD	190.	10	6	4	0	CHOCOc1cHcHcHcHc1COCHO	O=CC(=O)c1cccc1C(=O)C=O	0.551E-04	93.2
PhKG	166.	8	6	4	0	c1HcHcHcHcHc1COCO(OOH)	c1cccc1C(=O)C(=O)(OO)	0.149E-02	80.4
PhKKAnhy	204.	10	4	5	0	c12cHcHcHcHc1COCO-O-COC2O	c12cccc1C(=O)C(=O)OC(=O)C2=O	0.786E-07	121.8
PhKOA	180.	9	8	4	0	c1HcHcHcHcHc1COCH(OH)CO(OH)	c1cccc1C(=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)	ΔH ^{vap} (kJ)
PhKOAnhy	206.	10	6	5	0	c12cHcHcHcHc1COCH(OH)CO-O-C2O	c12cccc1C(=O)C(O)C(=O)OC2=O	0.174E-08	141.5
PhKOG	196.	9	8	5	0	c1HcHcHcHcHc1COCH(OH)CO(OOH)	c1cccc1C(=O)C(O)C(=O)(OO)	0.300E-05	110.3
PhKOEEst	224.	10	8	6	0	c12cHcHcHcHc1COCH(OH)CH(OOH)-O-C2O	c12cccc1C(=O)C(O)C(OO)OC2=O	0.132E-09	155.6
PhKOOEst	208.	10	8	5	0	c12cHcHcHcHc1COCH(OH)CH(OH)-O-C2O	c12cccc1C(=O)C(O)C(O)OC2=O	0.274E-08	141.3
PhKOP	241.	9	7	7	1	c1HcHcHcHcHc1COCH(OH)CO(OONO2)	c1cccc1C(=O)C(O)C(=O)(OON(=O)=O)	0.218E-04	99.6
PhKP	211.	8	5	6	1	c1HcHcHcHcHc1COCO(OONO2)	c1cccc1C(=O)C(=O)(OON(=O)=O)	0.338E-02	75.6
PhNA	197.	8	7	5	1	c1HcHcHcHcHc1CH(ONO2)CO(OH)	c1cccc1C(ON(=O)=O)C(=O)(O)	0.124E-04	103.9
PhNDKD	237.	10	7	6	1	CHOCO1cHcHcHcHc1CH(ONO2)CHO	O=CC(=O)c1cccc1C(ON(=O)=O)C=O	0.223E-05	109.2
PhNG	213.	8	7	6	1	c1HcHcHcHcHc1CH(ONO2)CO(OOH)	c1cccc1C(ON(=O)=O)C(=O)(OO)	0.494E-04	97.4
PhNP	258.	8	6	8	2	c1HcHcHcHcHc1CH(ONO2)CO(OONO2)	c1cccc1C(ON(=O)=O)C(=O)(OON(=O)=O)	0.186E-03	89.9
PhOA	152.	8	8	3	0	c1HcHcHcHcHc1CH(OH)CO(OH)	c1cccc1C(O)C(=O)(O)	0.182E-04	103.1
PhOCA	166.	9	10	3	0	c1HcHcHcHcHc1CH(OH)CH2CO(OH)	c1cccc1C(O)CC(=O)(O)	0.565E-05	108.2
PhOCAnhy	192.	10	8	4	0	c12cHcHcHcHc1CH(OH)CH2CO-O-C2O	c12cccc1C(O)CC(=O)OC2=O	0.129E-07	132.3
PhOCG	182.	9	10	4	0	c1HcHcHcHcHc1CH(OH)CH2CO(OOH)	c1cccc1C(O)CC(=O)(OO)	0.277E-04	100.9
PhOCHEst	210.	10	10	5	0	c12cHcHcHcHc1CH(OH)CH2CH(OOH)-O-C2O	c12cccc1C(O)CC(OO)OC2=O	0.263E-08	141.3
PhOCOESt	194.	10	10	4	0	c12cHcHcHcHc1CH(OH)CH2CH(OH)-O-C2O	c12cccc1C(O)CC(O)OC2=O	0.507E-07	127.5
PhOCP	227.	9	9	6	1	c1HcHcHcHcHc1CH(OH)CH2CO(OONO2)	c1cccc1C(O)CC(=O)(OON(=O)=O)	0.146E-03	92.0
PhOD	136.	8	8	2	0	c1HcHcHcHcHc1CH(OH)CHO	c1cccc1C(O)C=O	0.956E-02	73.7
PhODKD	192.	10	8	4	0	CHOCO1cHcHcHcHc1CH(OH)CHO	O=CC(=O)c1cccc1C(O)C=O	0.366E-05	107.7
PhOG	168.	8	8	4	0	c1HcHcHcHcHc1CH(OH)CO(OOH)	c1cccc1C(O)C(=O)(OO)	0.889E-04	95.9
PhOH	154.	8	10	3	0	c1HcHcHcHcHc1CH(OH)CH2(OOH)	c1cccc1C(O)C(OO)	0.428E-04	98.3
PhOKAnhy	206.	10	6	5	0	c12cHcHcHcHc1COCO-O-COC2H(OH)	c12cccc1C(=O)C(=O)OC(=O)C2(O)	0.174E-08	141.5
PhOKHEst	224.	10	8	6	0	c12cHcHcHcHc1COCH(OOH)-O-COC2H(OH)	c12cccc1C(=O)C(OO)OC(=O)C2(O)	0.132E-09	155.6
PhOKOESt	208.	10	8	5	0	c12cHcHcHcHc1COCH(OH)-O-COC2H(OH)	c12cccc1C(=O)C(O)OC(=O)C2(O)	0.274E-08	141.3
PhON	183.	8	9	4	1	c1HcHcHcHcHc1CH(OH)CH2(ONO2)	c1cccc1C(O)C(ON(=O)=O)	0.405E-03	88.3
PhOO	138.	8	10	2	0	c1HcHcHcHcHc1CH(OH)CH2(OH)	c1cccc1C(O)C(O)	0.489E-03	87.4
PhOOAnhy	194.	9	6	5	0	c12cHcHcHcHc1C(OH)(OH)CO-O-C2O	c12cccc1C(O)(O)C(=O)OC2=O	0.326E-06	117.5
PhOP	213.	8	7	6	1	c1HcHcHcHcHc1CH(OH)CO(OONO2)	c1cccc1C(O)C(=O)(OON(=O)=O)	0.438E-03	87.3
PhOUA	164.	9	8	3	0	c1HcHcHcHcHc1Cd(OH)=CdHCO(OH)	c1cccc1C(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)	ΔH ^{vap} (kJ)
PhOUAnhy	190.	10	6	4	0	c12cHcHcHcHc1Cd(OH)=CdHCO-O-C2O	c12cccc1C(O)=CC(=O)OC2=O	0.152E-07	131.5
PhOUG	180.	9	8	4	0	c1HcHcHcHc1Cd(OH)=CdHCO(OOH)	c1cccc1C(O)=CC(=O)(OO)	0.993E-05	105.5
PhOUHEst	208.	10	8	5	0	c12cHcHcHcHc1Cd(OH)=CdHCH(OOH)-O-C2O	c12cccc1C(O)=CC(OO)OC2=O	0.447E-08	138.9
PhOUOEst	192.	10	8	4	0	c12cHcHcHcHc1Cd(OH)=CdHCH(OH)-O-C2O	c12cccc1C(O)=CC(O)OC2=O	0.856E-07	125.3
PhOUP	225.	9	7	6	1	c1HcHcHcHc1Cd(OH)=CdHCO(OONO2)	c1cccc1C(O)=CC(=O)(OON(=O)=O)	0.604E-04	96.0
PhPA	227.	8	5	7	1	CO(OH)c1cHcHcHc1CO(OONO2)	C(=O)(O)c1cccc1C(=O)(OON(=O)=O)	0.572E-05	106.5
PhPD	211.	8	5	6	1	CHOc1cHcHcHc1CO(OONO2)	C(=O)c1cccc1C(=O)(OON(=O)=O)	0.190E-02	78.1
PhPKOA	285.	10	7	9	1	CO(OH)c1cHcHcHc1COCH(OH)CO(OONO2)	C(=O)(O)c1cccc1C(=O)C(O)C(=O)(OON(=O)=O)	0.212E-09	154.8
PhPKOD	269.	10	7	8	1	CO(OONO2)c1cHcHcHc1COCH(OH)CHO	C(=O)(OON(=O)=O)c1cccc1C(=O)C(O)C=O	0.253E-06	120.2
PhPND	286.	9	6	9	2	CO(OONO2)c1cHcHcHc1CH(OONO2)CHO	C(=O)(OON(=O)=O)c1cccc1C(O)C(=O)C=O	0.337E-05	107.8
PhPOCD	255.	10	9	7	1	CO(OONO2)c1cHcHcHc1CH(OH)CH2CHO	C(=O)(OON(=O)=O)c1cccc1C(O)CC=O	0.210E-05	110.8
PhPOKA	285.	10	7	9	1	CO(OH)CH(OH)c1cHcHcHc1COCO(OONO2)	C(=O)(O)C(O)c1cccc1C(=O)C(=O)(OON(=O)=O)	0.212E-09	154.8
PhPOKD	269.	10	7	8	1	CHOCOc1cHcHcHc1CH(OH)CO(OONO2)	O=CC(=O)c1cccc1C(O)C(=O)(OON(=O)=O)	0.253E-06	120.2
PhPOUA	269.	10	7	8	1	CO(OH)c1cHcHcHc1Cd(OH)=CdHCO(OONO2)	C(=O)(O)c1cccc1C(O)=CC(=O)(OON(=O)=O)	0.758E-09	149.2
PhPOUD	253.	10	7	7	1	CO(OONO2)c1cHcHcHc1Cd(OH)=CdHCHO	C(=O)(OON(=O)=O)c1cccc1C(O)=CC=O	0.806E-06	115.2
PhPUA1	253.	10	7	7	1	CO(OH)c1cHcHcHc1CdH=CdHCO(OONO2)	C(=O)(O)c1cccc1C=CC(=O)(OON(=O)=O)	0.115E-06	124.1
PhPUA2	253.	10	7	7	1	CO(OONO2)c1cHcHcHc1CdH=CdHCO(OH)	C(=O)(OON(=O)=O)c1cccc1C=CC(=O)(O)	0.115E-06	124.1
PhPUD1	237.	10	7	6	1	CO(OONO2)c1cHcHcHc1CdH=CdHCHO	C(=O)(OON(=O)=O)c1cccc1C=CC=O	0.541E-04	94.1
PhPUD2	237.	10	7	6	1	CHOc1cHcHcHc1CdH=CdHCO(OONO2)	C(=O)c1cccc1C=CC(=O)(OON(=O)=O)	0.645E-04	93.0
PhUA	148.	9	8	2	0	c1HcHcHcHc1CdH=CdHCO(OH)	c1cccc1C=CC(=O)(O)	0.176E-03	90.7
PhUAnhy	174.	10	6	3	0	c12cHcHcHcHc1CdH=CdHCO-O-C2O	c12cccc1C=CC(=O)OC2=O	0.195E-05	107.0
PhUG	164.	9	8	3	0	c1HcHcHcHc1CdH=CdHCO(OOH)	c1cccc1C=CC(=O)(OO)	0.718E-03	84.3
PhUHEst1	192.	10	8	4	0	c12cHcHcHcHc1CdH=CdHCH(OOH)-O-C2O	c12cccc1C=CC(OO)OC2=O	0.945E-06	111.7
PhUHEst2	192.	10	8	4	0	c12cHcHcHcHc1CdH=CdHCO-O-C2H(OOH)	c12cccc1C=CC(=O)OC2(OO)	0.694E-06	113.0
PhUOEst1	176.	10	8	3	0	c12cHcHcHcHc1CdH=CdHCH(OH)-O-C2O	c12cccc1C=CC(O)OC2=O	0.132E-04	99.6
PhUOEst2	176.	10	8	3	0	c12cHcHcHcHc1CdH=CdHCO-O-C2H(OH)	c12cccc1C=CC(=O)OC2(O)	0.974E-05	100.8
PhUP	209.	9	7	5	1	c1HcHcHcHc1CdH=CdHCO(OONO2)	c1cccc1C=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)	ΔH ^{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)	Name	MW (g mol ⁻¹)	Chem code (GECKO-A)
1DC	59.	CHOCH2(O.)	1PhDKOA	223.	CO(OH)c1cHcHcHcHc1COCH(OH)CO(O.)
1Na	143.	c12cHcHcHcHc1cHcHcHc2(O.)	1PhDKOD	207.	CO(O.)c1cHcHcHcHc1COCH(OH)CHO
1NaEpox	177.	c12cHcHcHcHc1C3H-O-C3HCH(OH)C2H(O.)	1PhDOCD	193.	CO(O.)c1cHcHcHcHc1CH(OH)CH2CHO
1NaKON	238.	c12cHcHcHcHc1CH(ONO2)CH(O.)CH(OH)C2O	1PhDOD	193.	CHOc1cHcHcHcHc1CH(O.)CH(OH)CHO
1NaO	159.	c12cHcHcHcHc1cHcHc(O.)c2(OH)	1PhDOKA	223.	CO(OH)CH(OH)c1cHcHcHcHc1COCO(O.)
1NaOBp	193.	c12cHcHcHcHc1CH(O.)C3HCH(OH)C2H-O--O3-	1PhDOKD	207.	CHOCoc1cHcHcHcHc1CH(OH)CO(O.)
1NaOEpox	193.	c12cHcHcHcHc1C3H-O-C3HCH(OH)C2(OH)(O.)	1PhDOOD	209.	CHOc1cHcHcHcHc1C(OH)(O.)CH(OH)CHO
1NaOKK	191.	c12cHcHcHcHc1CH(OH)CH(O.)COC2O	1PhDOOD1	209.	CHOc1cHcHcHcHc1C(OH)(OH)CH(O.)CHO
1NaOOBp	209.	c12cHcHcHcHc1CH(O.)C3HCH(OH)C2(OH)-O--O3-	1PhDOUA	207.	CO(OH)c1cHcHcHcHc1Cd(OH)=CdHCO(O.)
1NaOOK	193.	c12cHcHcHcHc1COCH(OH)CH(O.)C2H(OH)	1PhDOUD	191.	CO(O.)c1cHcHcHcHc1Cd(OH)=CdHCHO
1NaOOK2	193.	c12cHcHcHcHc1CH(OH)CH(O.)CH(OH)C2O	1PhDUA1	191.	CO(OH)c1cHcHcHcHc1CdH=CdHCO(O.)
1NaOOBp	225.	c12cHcHcHcHc1C(OH)(O.)C3HCH(OH)C2(OH)-O--O3-	1PhDUA2	191.	CO(O.)c1cHcHcHcHc1CdH=CdHCO(OH)
1NaOort	177.	c12cHcHcHcHc1CH(OH)CH(O.)CdH=Cd2(OH)	1PhDUD1	175.	CO(O.)c1cHcHcHcHc1CdH=CdHCHO
1NaOort	161.	c12cHcHcHcHc1CdH=CdHCH(O.)C2H(OH)	1PhDUD2	175.	CHOc1cHcHcHcHc1CdH=CdHCO(O.)
1NaOpar	161.	c12cHcHcHcHc1CH(O.)CdH=CdHC2H(OH)	1PhEst	149.	c12cHcHcHcHc1CO-O-C2H(O.)
1ONaEpox	193.	c12cHcHcHc(OH)c1C3H-O-C3HCH(OH)C2H(O.)	1PhKA	165.	c1(O.)cHcHcHcHc1COCO(OH)
1ONaOBp	209.	c12cHcHcHc(OH)c1CH(O.)C3HCH(OH)C2H-O--O3-	1PhKD	149.	c1HcHcHcHcHc1COCO(O.)
1ONaOOK	209.	c12cHcHcHc(OH)c1COCH(OH)CH(O.)C2H(OH)	1PhKKA	193.	c1(O.)cHcHcHcHc1COCOCO(OH)
1ONaOort	177.	c12cHcHcHc(OH)c1CdH=CdHCH(O.)C2H(OH)	1PhKOA	195.	c1(O.)cHcHcHcHc1COCH(OH)CO(OH)
1ONaOpar	177.	c12cHcHcHc(OH)c1CH(O.)CdH=CdHC2H(OH)	1PhKOD	179.	c1HcHcHcHcHc1COCH(OH)CO(O.)
1OPhDenol	193.	CHOc1cHcHcHc(OH)c1CH(O.)CdH=CdH(OH)	1PhKOEest	207.	c12cHcHcHcHc1COCH(OH)CH(O.)-O-C2O
1OPhDOD	209.	CHOc1cHcHcHc(OH)c1CH(O.)CH(OH)CHO	1PhO	137.	c1HcHcHcHcHc1CH(OH)CH2(O.)
1OPhDUA	207.	CO(OH)c1cHcHcHc(OH)c1CdH=CdHCO(O.)	1PhOA	167.	c1(O.)cHcHcHcHc1CH(OH)CO(OH)
1OPhDUD	191.	CO(O.)c1cHcHcHc(OH)c1CdH=CdHCHO	1PhOCD	165.	c1HcHcHcHcHc1CH(OH)CH2CO(O.)
1OPhUA	179.	c1(O.)cHcHcHc(OH)c1CdH=CdHCO(OH)	1PhOCEst	193.	c12cHcHcHcHc1CH(OH)CH2CH(O.)-O-C2O
1OPhUD	163.	c1HcHcHcHc(OH)c1CdH=CdHCO(O.)	1PhOD	151.	c1HcHcHcHcHc1CH(OH)CO(O.)
1OPhUEst	191.	c12cHcHcHc(OH)c1CdH=CdHCH(O.)-O-C2O	1PhOKEst	207.	c12cHcHcHcHc1COCH(O.)-O-COC2H(OH)
1Ph	93.	c1HcHcHcHcHc1(O.)	1PhOUA	179.	c1(O.)cHcHcHcHc1Cd(OH)=CdHCO(OH)
1PhA	137.	CO(OH)c1cHcHcHcHc1(O.)	1PhOUD	163.	c1HcHcHcHcHc1Cd(OH)=CdHCO(O.)
1PhAEnol	193.	CO(OH)c1cHcHcHcHc1CH(O.)CdH=CdH(OH)	1PhOUEst	191.	c12cHcHcHcHc1Cd(OH)=CdHCH(O.)-O-C2O
1PhAO	181.	CO(OH)c1cHcHcHcHc1CH(OH)CH2(O.)	1PhUA	163.	c1(O.)cHcHcHcHc1CdH=CdHCO(OH)
1PhAOCD	209.	CO(OH)c1cHcHcHcHc1CH(OH)CH2CO(O.)	1PhUD	147.	c1HcHcHcHcHc1CdH=CdHCO(O.)
1PhAOOD	225.	CO(OH)c1cHcHcHcHc1C(OH)(O.)CH(OH)CHO	1PhUEst1	175.	c12cHcHcHcHc1CdH=CdHCH(O.)-O-C2O
1PhD	121.	CHOc1cHcHcHcHc1(O.)	1PhUEst2	175.	c12cHcHcHcHc1CdH=CdHCO-O-C2H(O.)
1PhDA	165.	CO(OH)c1cHcHcHcHc1CO(O.)	2DC	75.	CHOCH2(OO.)
1PhDD	149.	CHOc1cHcHcHcHc1CO(O.)	2Na	159.	c12cHcHcHcHc1cHcHcHc2(OO.)
1PhDenol	177.	CHOc1cHcHcHcHc1CH(O.)CdH=CdH(OH)	2NaKON	254.	c12cHcHcHcHc1CH(ONO2)CH(OO.)CH(OH)C2O
1PhDKD	191.	CHOc1cHcHcHcHc1COCH(O.)CHO	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.	c12cHcHcHc1CH(OH)CH(OO.)COC2O
2NaOO	193.	c12cHcHcHc1CH(OH)CH(OO.)CdH=Cd2(OH) <i>-interm_par/ort-</i>
2NaOOBp	225.	c12cHcHcHc1CH(OO.)C3HCH(OH)C2(OH)-O--O3-
2NaOOK	209.	c12cHcHcHc1COCH(OH)CH(OO.)C2H(OH)
2NaOOK2	209.	c12cHcHcHc1CH(OH)CH(OO.)CH(OH)C2O
2NaOOO	209.	c12cHcHcHc1Cd(OH)=CdHCH(OH)C2(OH)(OO.)
2NaOOOBp	241.	c12cHcHcHc1C(OH)(OO.)C3HCH(OH)C2(OH)-O--O3-
2NaOOort	193.	c12cHcHcHc1CH(OH)CH(OO.)CdH=Cd2(OH)
2NaOort	177.	c12cHcHcHc1CdH=CdHCH(OO.)C2H(OH)
2NaOpar	177.	c12cHcHcHc1CH(OO.)CdH=CdHC2H(OH)
2ONaO	193.	c12cHcHcHc(OH)c1CdH=CdHCH(OO.)C2H(OH) <i>-interm_par/ort-</i>
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.	c1HcHcHcHc1(OO.)
2PhA	153.	CO(OH)c1cHcHcHc1(OO.)
2PhAO	197.	CO(OH)c1cHcHcHc1CH(OH)CH2(OO.)
2PhD	137.	CHOc1cHcHcHc1(OO.)
2PhDKD	207.	CHOc1cHcHcHc1COCH(OO.)CHO
2PhDOD	209.	CHOc1cHcHcHc1CH(OO.)CH(OH)CHO
2PhDOOD	225.	CHOc1cHcHcHc1C(OH)(OH)CH(OO.)CHO
2PhEst	165.	c12cHcHcHc1CO-O-C2H(OO.)
2PhKA	181.	c1(OO.)cHcHcHc1COCOC(OH)
2PhKKA	209.	c1(OO.)cHcHcHc1COCOC(OH)
2PhKOA	211.	c1(OO.)cHcHcHc1COCH(OH)CO(OH)
2PhKOESt	223.	c12cHcHcHc1COCH(OH)CH(OO.)-O-C2O
2PhO	153.	c1HcHcHcHc1CH(OH)CH2(OO.)
2PhOA	183.	c1(OO.)cHcHcHc1CH(OH)CO(OH)
2PhOCEst	209.	c12cHcHcHc1CH(OH)CH2CH(OO.)-O-C2O
2PhOKESt	223.	c12cHcHcHc1COCH(OO.)-O-COC2H(OH)
2PhOUA	195.	c1(OO.)cHcHcHc1Cd(OH)=CdHCO(OH)
2PhOUEst	207.	c12cHcHcHc1Cd(OH)=CdHCH(OO.)-O-C2O
2PhUA	179.	c1(OO.)cHcHcHc1CdH=CdHCO(OH)
2PhUEst1	191.	c12cHcHcHc1CdH=CdHCH(OO.)-O-C2O
2PhUEst2	191.	c12cHcHcHc1CdH=CdHCO-O-C2H(OO.)
3GLY	89.	CHOCO(OO.)

Name	MW (g mol ⁻¹)	Chem code (GECKO-A)
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)c1cHcHcHc1CO(OO.)
3PhAOC	225.	CO(OH)c1cHcHcHc1CH(OH)CH2CO(OO.)
3PhD	165.	CHOc1cHcHcHc1CO(OO.)
3PhK	165.	c1HcHcHcHc1COCO(OO.)
3PhKO	195.	c1HcHcHcHc1COCH(OH)CO(OO.)
3PhKOA	239.	CO(OH)c1cHcHcHc1COCH(OH)CO(OO.)
3PhKOD	223.	CO(OO.)c1cHcHcHc1COCH(OH)CHO
3PhN	212.	c1HcHcHcHc1CH(ONO2)CO(OO.)
3PhND	240.	CO(OO.)c1cHcHcHc1CH(ONO2)CHO
3PhO	167.	c1HcHcHcHc1CH(OH)CO(OO.)
3PhOC	181.	c1HcHcHcHc1CH(OH)CH2CO(OO.)
3PhOCD	209.	CO(OO.)c1cHcHcHc1CH(OH)CH2CHO
3PhOKA	239.	CO(OH)CH(OH)c1cHcHcHc1COCO(OO.)
3PhOKD	223.	CHOCc1cHcHcHc1CH(OH)CO(OO.)
3PhOU	179.	c1HcHcHcHc1Cd(OH)=CdHCO(OO.)
3PhOUA	223.	CO(OH)c1cHcHcHc1Cd(OH)=CdHCO(OO.)
3PhOUD	207.	CO(OO.)c1cHcHcHc1Cd(OH)=CdHCHO
3PhU	163.	c1HcHcHcHc1CdH=CdHCO(OO.)
3PhUA1	207.	CO(OH)c1cHcHcHc1CdH=CdHCO(OO.)
3PhUA2	207.	CO(OO.)c1cHcHcHc1CdH=CdHCO(OH)
3PhUD1	191.	CO(OO.)c1cHcHcHc1CdH=CdHCHO
3PhUD2	191.	CHOc1cHcHcHc1CdH=CdHCO(OO.)
4NaO	145.	c12cHcHcHc1CdH=CdHC.HC2H(OH)
4NaOBp	177.	c12cHcHcHc1CH.C3HCH(OH)C2H-O--O3-
4NaOOBp	193.	c12cHcHcHc1CH.C3HCH(OH)C2(OH)-O--O3-
4NaOPEN1	159.	C.Oc1cHcHcHc1CdH=CdHCHO
4NaOPEN2	159.	CHOc1cHcHcHc1CdH=CdHC.O
4NaOPENO	177.	C.Oc1cHcHcHc1CH(OH)CH2CHO
4NaOPENOL	175.	C.Oc1cHcHcHc1Cd(OH)=CdHCHO
4ONaOBp	193.	c12cHcHcHc(OH)c1CH.C3HCH(OH)C2H-O--O3-
4ONaOPEN	175.	C.Oc1cHcHcHc(OH)c1CdH=CdHCHO
4PhDKOD	191.	C.Oc1cHcHcHc1COCH(OH)CHO
4PhODKD	191.	C.Oc1cHcHcHc1CH(OH)CHO
5OPhDCrg	180.	CHOc1cHcHcHc(OH)c1CH2C.H(OO.)
5PhDCrg	164.	CHOc1cHcHcHc1CH2C.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 PhDKKD + 0.18 HO2	ARR1	3.56E-11
B2-013	PhODKD + NO3 → PhDKKD + 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 PhKKAAnhy + 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	PhKKAAnhy	→ 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 PhKOAAnhy + 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 PhKOAAnhy + 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 R02) 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	→ 1PhA OCD + NO2	ARR2	7.50E-12	-290.0
B4-018	3PhAOC + NO2	→ PhA OCP	ARR3	6.143E-09	-1.1 0.0
B4-019	3PhAOC + NO3	→ 1PhA OCD + NO2	ARR2	8.90E-12	305.0
B4-020	3PhAOC + HO2	→ 0.65 PhA OCG + 0.15 PhA OCA + 0.20 1PhA OCD + 0.15 O3 + 0.20 HO	ARR2	3.324E-12	-730.0
B4-021	3PhAOC + MO2	→ 0.80 1PhA OCD + 0.20 PhA OCA + CH2O + 0.80 HO2	ARR2	2.000E-12	-508.0
B4-022	1PhA OCD	→ 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 PhA ON	ARR2	2.7E-12	-360.0
B4-024	2PhAO + NO3	→ 1PhAO + NO2	ARR2	8.90E-12	390.0
B4-025	2PhAO + HO2	→ PhA OH	ARR2	2.623E-13	-1300.0
B4-026	2PhAO + MO2	→ 0.60 1PhAO + 0.20 PhA OO + 0.20 PhA OD + 0.60 HO2 + 0.80 CH2O + 0.20 MOH	ARR2	1.03E-13	-1038.0
B4-027	1PhAO	→ PhA OD + 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 R02)

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	→ OHPPhUA	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	

BLOCK 5.4: 4NaOOBp CHEMISTRY (PEROXY 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

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	

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

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

B9-009	NaOOp _{ar} + HO	→	ARR1	3.29E-10	
B9-010	NaOOp _{ar} + O ₃	→	ARR1	3.67E-16	
B9-011	NaOOp _{ar} + NO ₃	→	ARR1	2.73E-13	
B9-012	NaOKp _{ar} + O ₃	→	ARR1	5.24E-18	
B9-013	NaOKp _{ar} + NO ₃	→	ARR1	7.96E-15	
B9-014	NaQuin + HO	→	ARR1	3.17E-11	
B9-015	NaNOOK + HO	→	ARR1	8.13E-12	
B9-016	NaNOOK + NO ₃	→	ARR1	5.30E-15	
B9-017	NaHOOK + HO	→	ARR1	4.11E-11	
B9-018	NaHOOK + NO ₃	→	ARR1	5.30E-15	
B9-019	NaOOOK + HO	→	ARR1	4.93E-11	
B9-020	NaOOOK + NO ₃	→	ARR1	9.95E-15	
B9-021	NaOOKK + HO	→	ARR1	1.13E-11	
B9-022	NaOOKK + NO ₃	→	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 + NO ₂	ARR2	5.20E+16	13850.00
B9-028	PhPOKD + HO	→	ARR1	1.80E-11	
B9-029	PhPOKD	→ 3PhOKD + NO ₂	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 + NO ₂	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 + NO ₂	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 + NO ₃	→	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	PhKOAAnhy + 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 + NO ₂	ARR2	5.20E+16	13850.00
B9-059	PhPKOD + HO	→	ARR1	1.94E-11	
B9-060	PhPKOD	→ 3PhKOD + NO ₂	ARR2	5.20E+16	13850.00
B9-061	PhPKOD + NO ₃	→	ARR1	1.85E-13	
B9-062	PhGKOD + HO	→	ARR1	2.25E-11	
B9-063	PhGKOD + NO ₃	→	ARR1	1.85E-13	
B9-064	PhAKOD + HO	→	ARR1	2.00E-11	
B9-065	PhAKOD + NO ₃	→	ARR1	1.85E-13	
B9-066	PhAKD + HO	→	ARR1	1.46E-11	
B9-067	OPhKOA + HO	→	ARR1	8.43E-12	
B9-068	PhKOP	→ 3PhKO + NO ₂	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	

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	

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	OHPPhUA + 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	

M02 (CH3O2.) and MOH (CH3OH) are species from RACM2

Table S4: kinetics.

kinetic type	formula
<i>ARR1</i>	$k = x_1$
<i>ARR1(XX)</i>	$k = x_1 [XX]$
<i>ARR2</i>	$k = x_1 e^{\frac{-x_2}{T}}$
<i>ARR2(XX)</i>	$k = x_1 e^{\frac{-x_2}{T}} [XX]$
<i>ARR3</i>	$k = x_1 T^{x_2} e^{\frac{-x_3}{T}}$
<i>PHOTO</i>	$k = x_1$ (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 $\mu\text{g}/\text{m}^3$).

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	NaOOpair	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	HPPhUA	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	HPPhKA	0	0
184	VOPhA	0.152	0.388
185	HPPhOA	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	PhAOD	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	NaOOKK	0	0
195	OPhKKA	0	0
197	HPPhOUA	0	0
197	OHPPhUA	0	0
197	PhKOG	0	0
197	PhAHD	0	0
197	HPPhEpoxA	0	0

m/z	species	Gas	Part.
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	HPPhKKA	0	0
211	ONaOOKK	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	HPPhKOA	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	NaOOOBp	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