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Development of a detailed gaseous oxidation scheme of naphthalene for secondary organic aerosol (SOA) formation and speciation

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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
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
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
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)	ΔH^{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)	ΔH^{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)	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
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
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
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
PhAKA	194.	9	6	5	0	CO(OH)COc1cHcHcHcHc1CO(OH)	C(=O)(O)C(=O)c1ccccc1C(=O)(O)	1.909E-07	121.5
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)	ΔH^{vap} (kJ)
PhAOA	196.	9	8	5	0	CO(OH)c1cHcHcHcHc1CH(OH)CO(OH)	C(=O)(O)c1ccccc1C(O)C(=O)(O)	3.809E-10	149.5
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

Name	MW (g mol^{-1})	nbC	nbH	nbO	nbN	Chem code (GECKO-A)	Smile code	P^{sat} (torr)	ΔH^{vap} (kJ)
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
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
PhGOA	212.	9	8	6	0	CO(OH)c1cHcHcHcHc1CH(OH)CO(OOH)	C(=O)(O)c1ccccc1C(O)C(=O)(OO)	3.809E-09	138.7
PhGOCD	210.	10	10	5	0	CO(OOH)c1cHcHcHcHc1CH(OH)CH2CHO	C(=O)(OO)c1ccccc1C(O)CC=O	0.254E-06	121.7
PhGOD	196.	9	8	5	0	CHOCH(OH)c1cHcHcHcHc1CO(OOH)	O=CC(O)c1ccccc1C(=O)(OO)	0.120E-05	110.8
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
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

Name	MW ($g\ mol^{-1}$)	nbC	nbH	nbO	nbN	Chem code (GECKO-A)	Smile code	P^{sat} (torr)	ΔH^{vap} (kJ)
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
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
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
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
PhOAnhy	178.	9	6	4	0	c12cHcHcHcHc1CH(OH)CO-O-C2O	c12ccccc1C(O)C(=O)OC2=O	0.120E-03	90.5
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
PhOHEst	196.	9	8	5	0	c12cHcHcHcHc1CO-O-CH(OOH)C2H(OH)	c12ccccc1C(=O)OC(OO)C2(O)	9.568E-09	135.6

Name	MW (g mol^{-1})	nbC	nbH	nbO	nbN	Chem code (GECKO-A)	Smile code	P^{sat} (torr)	ΔH^{vap} (kJ)
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
PhOOEst	180.	9	8	4	0	c12cHcHcHcHc1CO-O-CH(OH)C2H(OH)	c12ccccc1C(=O)OC(O)C2(O)	1.909E-07	121.3
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
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
PhPOA	257.	9	7	8	1	CO(OH)c1cHcHcHcHc1CH(OH)CO(OONO2)	C(=O)(O)c1ccccc1C(O)C(=O)(OON(=O)=O)	9.568E-09	135.8
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
PhPOD	241.	9	7	7	1	CHOCH(OH)c1cHcHcHcHc1CO(OONO2)	O=CC(O)c1ccccc1C(=O)(OON(=O)=O)	0.760E-05	105.2
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

Name	MW (g mol^{-1})	nbC	nbH	nbO	nbN	Chem code (GECKO-A)	Smile code	P^{sat} (torr)	ΔH^{vap} (kJ)
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
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
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
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
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
1PhDOA	195.	CO(OH)c1cHcHcHcHc1CH(OH)CO(O.)
1PhDOCD	193.	CO(O.)c1cHcHcHcHc1CH(OH)CH2CHO
1PhDOD	193.	CHOc1cHcHcHcHc1CH(O.)CH(OH)CHO
1PhDODb	179.	CO(O.)c1cHcHcHcHc1CH(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.)
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.)
1PhOCD	165.	c1HcHcHcHcHc1CH(OH)CH2CO(O.)
1PhOCEst	193.	c12cHcHcHcHc1CH(OH)CH2CH(O.)-O-C2O
1PhOD	151.	c1HcHcHcHcHc1CH(OH)CO(O.)
1PhOEst	179.	c12cHcHcHcHc1CO-O-CH(O.)C2H(OH)
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
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.)
2PhKOA	211.	c1(OO.)cHcHcHcHc1COCH(OH)CO(OH)
2PhKOEst	223.	c12cHcHcHcHc1COCH(OH)CH(OO.)-O-C2O
2PhO	153.	c1HcHcHcHcHc1CH(OH)CH2(OO.)
2PhOCEst	209.	c12cHcHcHcHc1CH(OH)CH2CH(OO.)-O-C2O
2PhOEst	195.	c12cHcHcHcHc1CO-O-CH(OO.)C2H(OH)
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.)

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)c1cHcHcHcHc1CO(OO.)
3PhAOC	225.	CO(OH)c1cHcHcHcHc1CH(OH)CH2CO(OO.)
3PhD	165.	CHOc1cHcHcHcHc1CO(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.)
3PhOA	211.	CO(OH)c1cHcHcHcHc1CH(OH)CO(OO.)
3PhOC	181.	c1HcHcHcHcHc1CH(OH)CH2CO(OO.)
3PhOD	195.	CO(OO.)c1cHcHcHcHc1CH(OH)CHO
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
4PhDOD	163.	C.Oc1cHcHcHcHc1CH(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	→	0.41 4PhODKD + 0.41 4PhDOD + 0.18 PhKDKD + 0.18 HO2 + 0.41 CO	*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 + 0.40 PhDKA + 0.4 CO2 + 0.4 HO2	*ARR1*	1.00E+06			
B2-031	1PhDOKD	→	0.60 PhOKAnhy + 0.60 HO2 + 0.40 PhKDD + 0.40 CO2 + 0.40 HO2	*ARR1*	1.00E+06			
B2-032	4PhDOD	→	0.40 2PhOEst + 0.60 3PhOD	*ARR1*	1.00E+06			
B2-033	2PhOEst + NO	→	1PhOEst + NO2	*ARR2*	2.7E-12	-360.0		
B2-034	2PhOEst + HO2	→	0.540 PhOHEst + 0.460 PhOAnhy + 0.20 HO + 0.20 HO2	*ARR2*	2.62E-13	-1300.0		
B2-035	2PhOEst + NO3	→	1PhOEst + NO2	*ARR2*	8.90E-12	390.0		
B2-036	2PhOEst + MO2	→	0.60 1PhOEst + 0.20 PhOAnhy + 0.20 PhOOEst + 0.60 HO2 + 0.80 CH2O + 0.20 MOH	*ARR2*	1.03E-13	-955.0		
B2-037	1PhOEst	→	3PhOA	*ARR3*	8.00E+10	1.7	3723.0	
B2-038	3PhOA + NO	→	1PhDOA + NO2	*ARR2*	7.50E-12	-290.0		
B2-039	3PhOA + NO2	→	PhPOA	*ARR3*	6.143E-09	-1.1	0.0	
B2-040	3PhOA + NO3	→	1PhDOA + NO2	*ARR2*	8.90E-12	305.0		
B2-041	3PhOA + HO2	→	0.65 PhGOA + 0.15 PhAOA + 0.20 1PhDOA + 0.15 O3 + 0.20 HO	*ARR2*	3.324E-12	-730.0		
B2-042	3PhOA + MO2	→	0.80 1PhDOA + 0.20 PhAOA + CH2O + 0.80 HO2	*ARR2*	2.000E-12	-508.0		
B2-043	3PhOD + NO	→	1PhDODb + NO2	*ARR2*	7.50E-12	-290.0		
B2-044	3PhOD + NO2	→	PhPOD	*ARR3*	6.143E-09	-1.1	0.0	
B2-045	3PhOD + NO3	→	1PhDODb + NO2	*ARR2*	8.90E-12	305.0		
B2-046	3PhOD + HO2	→	0.65 PhGOD + 0.15 PhAOD + 0.20 1PhDODb + 0.15 O3 + 0.20 HO	*ARR2*	3.324E-12	-730.0		
B2-047	3PhOD + MO2	→	0.80 1PhDODb + 0.20 PhAOD + CH2O + 0.80 HO2	*ARR2*	2.000E-12	-508.0		
B2-048	1PhDOA	→	0.60 PhOAnhy + 0.60 HO + 0.40 PhAD + 0.4 CO2 + 0.4 HO2	*ARR1*	1.00E+06			
B2-049	1PhDODb	→	0.60 PhOAnhy + 0.60 HO2 + 0.40 PhD + 0.40 CO2 + 0.40 HO2 + 0.40 CO	*ARR1*	1.00E+06			
B2-050	3PhO + NO	→	1PhOD + NO2	*ARR2*	7.50E-12	-290.0		
B2-051	3PhO + NO2	→	PhOP	*ARR3*	6.143E-09	-1.1	0.0	
B2-052	3PhO + NO3	→	1PhOD + NO2	*ARR2*	8.90E-12	305.0		
B2-053	3PhO + HO2	→	0.65 PhOG + 0.15 PhOA + 0.20 1PhOD + 0.15 O3 + 0.20 HO	*ARR2*	3.324E-12	-730.0		
B2-054	3PhO + MO2	→	0.80 1PhOD + 0.20 PhOA + CH2O + 0.80 HO2	*ARR2*	2.000E-12	-508.0		
B2-055	1PhOD	→	PhD + CO2 + HO2	*ARR1*	1.00E+06			
B2-056	PhOKAnhy	→	PhAOKA	*ARR1(H2O)*	2.50E-22			
B2-057	PhOAnhy	→	PhAOA	*ARR1(H2O)*	2.50E-22			
B2-058	PhKDKD + HO	→	0.6 PhKAnhy + 0.24 HO + 0.36 HO2 + 0.16 3PhA + 0.16 CO + 0.16 CO2 + 0.24 3Ph + 0.48 CO + 0.24 CO2 + 0.6 CO	*ARR1*	2.59E-11			
B2-070	PhKAnhy	→	PhAKA	*ARR1(H2O)*	2.50E-22			
B2-059	PhKKAnhy	→	PhKAKA	*ARR1(H2O)*	2.50E-22			
B2-060	PhDKOD + HO	→	0.82 4PhDKOD + 0.18 PhDKKD + 0.18 HO2	*ARR1*	3.04E-11			
B2-061	PhDKOD + NO3	→	PhDKKD + HNO3 + HO2	*ARR1*	1.92E-13			
B2-062	4PhDKOD	→	0.40 2PhKOEst + 0.60 3PhKOD	*ARR1*	1.00E+06			
B2-063	2PhKOEst + NO	→	1PhKOEst + NO2	*ARR2*	2.7E-12	-360.0		
B2-064	2PhKOEst + HO2	→	0.540 PhKOHEst + 0.460 PhKOAnhy + 0.20 HO + 0.20 HO2	*ARR2*	2.62E-13	-1300.0		
B2-065	2PhKOEst + NO3	→	1PhKOEst + NO2	*ARR2*	8.90E-12	390.0		
B2-066	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		
B2-067	1PhKOEst	→	3PhKOA	*ARR3*	8.00E+10	1.7	3723.0	
B2-068	3PhKOA + NO	→	1PhDKOA + NO2	*ARR2*	7.50E-12	-290.0		
B2-069	3PhKOA + NO2	→	PhPKOA	*ARR3*	6.143E-09	-1.1	0.0	
B2-070	3PhKOA + NO3	→	1PhDKOA + NO2	*ARR2*	8.90E-12	305.0		
B2-071	3PhKOA + HO2	→	0.65 PhGKOA + 0.15 PhAKOA + 0.20 1PhDKOA + 0.15 O3 + 0.20 HO	*ARR2*	3.324E-12	-730.0		
B2-072	3PhKOA + MO2	→	0.80 1PhDKOA + 0.20 PhAKOA + CH2O + 0.80 HO2	*ARR2*	2.000E-12	-508.0		
B2-073	3PhKOD + NO	→	1PhDKOD + NO2	*ARR2*	7.50E-12	-290.0		
B2-074	3PhKOD + NO2	→	PhPKOD	*ARR3*	6.143E-09	-1.1	0.0	

B2-075	3PhKOD + NO3	→	1PhDKOD + NO2	*ARR2*	8.90E-12 305.0
B2-076	3PhKOD + HO2	→	0.65 PhGKOD + 0.15 PhAKOD + 0.20 1PhDKOD + 0.15 O3 + 0.20 HO	*ARR2*	3.324E-12 -730.0
B2-077	3PhKOD + MO2	→	0.80 1PhDKOD + 0.20 PhAKOD + CH2O + 0.80 HO2	*ARR2*	2.000E-12 -508.0
B2-078	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
B2-079	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
B2-080	2PhKOA + NO	→	1PhKOA + NO2	*ARR2*	2.7E-12 -360.0
B2-081	2PhKOA + NO2	→	1PhKOA + NO3	*ARR3*	6.143E-09 -1.1 0.0
B2-082	2PhKOA + NO3	→	1PhKOA + NO2	*ARR2*	8.90E-12 390.0
B2-083	2PhKOA + HO2	→	HPhKOA	*ARR2*	2.335E-13 -1300.0
B2-084	2PhKOA + MO2	→	0.80 1PhKOA + 0.20 OPhKOA + CH2O + 0.80 HO2	*ARR2*	1.03E-13 -398.0
B2-085	1PhKOA + O3	→	2PhKOA	*ARR1*	2.86E-13
B2-086	1PhKOA + NO2	→	VOPhKOA	*ARR1*	2.08E-12
B2-087	1PhKOA + HO2	→	OPhKOA	*ARR1*	2.30E-13
B2-088	3PhKO + NO	→	1PhKOD + NO2	*ARR2*	7.50E-12 -290.0
B2-089	3PhKO + NO2	→	PhKOP	*ARR3*	6.143E-09 -1.1 0.0
B2-090	3PhKO + NO3	→	1PhKOD + NO2	*ARR2*	8.90E-12 305.0
B2-091	3PhKO + HO2	→	0.65 PhKOG + 0.15 PhKOA + 0.20 1PhKOD + 0.15 O3 + 0.20 HO	*ARR2*	3.324E-12 -730.0
B2-092	3PhKO + MO2	→	0.80 1PhKOD + 0.20 PhKOA + CH2O + 0.80 HO2	*ARR2*	2.000E-12 -508.0
B2-093	1PhKOD	→	PhKD + CO2 + HO2	*ARR1*	1.00E+06
B2-094	PhKOAnhy	→	PhAKOA	*ARR1(H2O)*	2.50E-22
B2-095	PhDKKD + HO	→	0.20 2PhEst + 0.30 3PhD + CO + 0.3 PhKKAnhy + 0.12 HO + 0.18 HO2 + 0.08 3PhA + 0.08 CO + 0.08 CO2 + 0.12 3Ph + 0.24 CO + 0.12 CO2 + 0.3 CO	*ARR1*	2.51E-11
B2-096	PhKDD + HO	→	0.20 2PhEst + 0.30 3PhD + 0.5 CO + 0.3 PhKAnhy + 0.12 HO + 0.18 HO2 + 0.08 3PhA + 0.08 CO + 0.08 CO2 + 0.12 3Ph + 0.24 CO + 0.12 CO2 + 0.3 CO	*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
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*	1.12E+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*	1.12E+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*	1.12E+09 1.7 2301.7
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*	1.12E+09 1.7 2301.7
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	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		
B9-036	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	PhOHEst + HO	→		*ARR1*	1.95E-11		
B9-043	PhOAnhy + HO	→		*ARR1*	6.40E-12		
B9-044	PhOOEst + HO	→		*ARR1*	1.66E-11		
B9-045	PhPOA + HO	→		*ARR1*	7.27E-12		
B9-046	PhPOA	→	3PhOKA + NO2	*ARR2*	5.20E+16	13850.00	
B9-047	PhPOD + HO	→		*ARR1*	1.80E-11		
B9-048	PhPOD	→	3PhOKD + NO2	*ARR2*	5.20E+16	13850.00	
B9-049	PhGOD + HO	→		*ARR1*	2.59E-11		
B9-050	PhAOD + HO	→		*ARR1*	2.02E-11		
B9-051	PhKAKA + HO	→		*ARR1*	3.55E-13		
B9-052	PhKOHEst + HO	→		*ARR1*	1.95E-11		
B9-053	PhKOAnhy + HO	→		*ARR1*	6.40E-12		
B9-054	PhKOOEst + HO	→		*ARR1*	1.66E-11		
B9-055	PhPKOA + HO	→		*ARR1*	2.42E-12		
B9-056	PhPKOA	→	3PhKOA + NO2	*ARR2*	5.20E+16	13850.00	
B9-057	PhPKOD + HO	→		*ARR1*	1.94E-11		
B9-058	PhPKOD	→	3PhKOD + NO2	*ARR2*	5.20E+16	13850.00	
B9-059	PhPKOD + NO3	→		*ARR1*	1.85E-13		
B9-060	PhGKOD + HO	→		*ARR1*	2.25E-11		
B9-061	PhGKOD + NO3	→		*ARR1*	1.85E-13		
B9-062	PhAKOD + HO	→		*ARR1*	2.00E-11		
B9-063	PhAKOD + NO3	→		*ARR1*	1.85E-13		
B9-064	PhAKD + HO	→		*ARR1*	1.46E-11		
B9-065	OPhKOA + HO	→		*ARR1*	8.43E-12		
B9-066	PhKOP	→	3PhKO + NO2	*ARR2*	5.20E+16	13850.00	
B9-067	PhKOP + HO	→		*ARR1*	1.18E-12		
B9-068	PhKOG + HO	→		*ARR1*	9.10E-12		
B9-069	PhKOA + HO	→		*ARR1*	3.34E-12		
B9-070	PhKD + HO	→		*ARR1*	1.34E-11		
B9-071	PhKAnhy + HO	→		*ARR1*	3.12E-13		
B9-072	NaONort + HO	→		*ARR1*	9.16E-11		
B9-073	NaONort + O3	→		*ARR1*	8.24E-18		
B9-074	NaONort + NO3	→		*ARR1*	3.43E-13		
B9-075	NaOHort + HO	→		*ARR1*	2.26E-10		
B9-076	NaOHort + O3	→		*ARR1*	1.87E-16		
B9-077	NaOHort + NO3	→		*ARR1*	3.43E-13		
B9-078	NaOOort + HO	→		*ARR1*	2.65E-10		
B9-079	NaOOort + O3	→		*ARR1*	2.62E-16		
B9-080	NaOOort + NO3	→		*ARR1*	3.09E-13		
B9-081	PhDCD + HO	→		*ARR1*	4.06E-11		
B9-082	PhDCA + HO	→		*ARR1*	1.99E-11		
B9-083	PhDNOD + HO	→		*ARR1*	2.87E-11		
B9-084	PhDNOD + NO3	→		*ARR1*	4.55E-13		
B9-085	PhDHOD + HO	→		*ARR1*	5.09E-11		
B9-086	PhDHOD + NO3	→		*ARR1*	4.55E-13		
B9-087	PhDOOD + HO	→		*ARR1*	6.03E-11		
B9-088	PhDOOD + NO3	→		*ARR1*	4.58E-13		
B9-089	PhUAnhy + HO	→		*ARR2*	0.622E-11	-540.0	
B9-090	PhUAnhy + O3	→		*ARR1*	1.80E-16		
B9-091	PhUAnhy + NO3	→		*ARR1*	0.272E-14		
B9-092	PhUHEst1 + HO	→	0.5 PhUAnhy	*ARR1*	1.17E-10		
B9-093	PhUHEst1 + O3	→		*ARR1*	9.00E-15		
B9-094	PhUHEst1 + NO3	→		*ARR1*	3.40E-13		
B9-095	PhUOEst1 + HO	→	0.5 PhUAnhy	*ARR1*	1.25E-10		
B9-096	PhUOEst1 + O3	→		*ARR1*	1.26E-14		
B9-097	PhUOEst1 + NO3	→		*ARR1*	3.05E-13		
B9-098	PhPUA1 + HO	→		*ARR1*	5.17E-11		

B9-099	PhPUA1	→	3PhUA1 + NO2	*ARR2*	5.20E+16	13850.00
B9-100	PhGUA1 + HO	→	0.1 3PhUA1	*ARR1*	5.48E-11	
B9-101	PhGUA1 + NO3	→		*ARR1*	3.40E-13	
B9-102	PhAUA + HO	→		*ARR1*	5.23E-11	
B9-103	PhAUA + NO3	→		*ARR1*	3.40E-13	
B9-104	PhPUD1 + HO	→		*ARR1*	5.87E-11	
B9-105	PhPUD1	→	3PhUD1 + NO2	*ARR2*	5.20E+16	13850.00
B9-106	PhGUD1 + HO	→	0.1 3PhUD1	*ARR1*	6.18E-11	
B9-107	PhAUD1 + HO	→	0.25 3PhUA1	*ARR1*	5.92E-11	
B9-108	PhUP	→	3PhU + NO2	*ARR2*	5.20E+16	13850.00
B9-109	PhUP + HO	→		*ARR1*	4.39E-11	
B9-110	PhUG + HO	→		*ARR1*	4.70E-11	
B9-111	PhUG + NO3	→		*ARR1*	3.40E-13	
B9-112	PhUA + HO	→		*ARR1*	4.45E-11	
B9-113	PhUA + NO3	→		*ARR1*	3.40E-13	
B9-114	PhUHEst2 + HO	→	0.5 PhUAnhy	*ARR1*	1.17E-10	
B9-115	PhUHEst2 + O3	→		*ARR1*	9.00E-15	
B9-116	PhUHEst2 + NO3	→		*ARR1*	3.40E-13	
B9-117	PhUOEst2 + HO	→	0.5 PhUAnhy	*ARR1*	1.25E-10	
B9-118	PhUOEst2 + O3	→		*ARR1*	1.26E-14	
B9-119	PhUOEst2 + NO3	→		*ARR1*	3.05E-13	
B9-120	PhPUA2 + HO	→		*ARR1*	5.17E-11	
B9-121	PhPUA2	→	3PhUA2 + NO2	*ARR2*	5.20E+16	13850.00
B9-122	PhGUA2 + HO	→	0.1 3PhUA2	*ARR1*	5.48E-11	
B9-123	PhGUA2 + NO3	→		*ARR1*	3.40E-13	
B9-124	HPhUA + HO	→		*ARR1*	6.18E-11	
B9-125	OPhUA + HO	→		*ARR1*	1.01E-10	
B9-126	VOPhUA + HO	→		*ARR1*	7.00E-11	
B9-127	PhPUD2 + HO	→		*ARR1*	5.87E-11	
B9-128	PhPUD2	→	3PhUD2 + NO2	*ARR2*	5.20E+16	13850.00
B9-129	PhGUD2 + HO	→	0.1 3PhUD2	*ARR1*	6.18E-11	
B9-130	PhAUD2 + HO	→	0.25 3PhUA2	*ARR1*	5.92E-11	
B9-131	NaONBp + HO	→		*ARR1*	5.38E-11	
B9-132	NaONBp + NO3	→		*ARR1*	1.91E-13	
B9-133	NaOHBp + HO	→		*ARR1*	7.27E-11	
B9-134	NaOHBp + NO3	→		*ARR1*	1.91E-13	
B9-135	NaOOBp + HO	→		*ARR1*	1.04E-10	
B9-136	NaOOBp + NO3	→		*ARR1*	2.08E-13	
B9-137	NaOKBp + HO	→		*ARR1*	2.70E-11	
B9-138	NaOKBp + NO3	→		*ARR1*	1.89E-13	
B9-139	PhOCHEst + HO	→		*ARR1*	3.67E-11	
B9-140	PhOCAnhy + HO	→		*ARR1*	2.52E-11	
B9-141	PhOCOEst + HO	→		*ARR1*	3.67E-11	
B9-142	PhAOCP	→	3PhAOC + NO2	*ARR2*	5.20E+16	13850.00
B9-143	PhAOCP + HO	→		*ARR1*	5.43E-11	
B9-144	PhAOCG + HO	→		*ARR1*	5.93E-11	
B9-145	PhAOCA + HO	→		*ARR1*	6.28E-11	
B9-146	PhAON + HO	→		*ARR1*	4.91E-11	
B9-147	PhAOH + HO	→		*ARR1*	6.28E-11	
B9-148	PhAOO + HO	→		*ARR1*	6.90E-11	
B9-149	PhAOD + HO	→		*ARR1*	6.50E-11	
B9-150	PhAOD + NO3	→		*ARR1*	2.74E-13	
B9-151	PhPOCD	→	3PhOCD + NO2	*ARR2*	5.20E+16	13850.00
B9-152	PhPOCD + HO	→		*ARR1*	7.57E-11	
B9-153	PhGOCD + HO	→		*ARR1*	7.88E-11	
B9-154	PhAOCD + HO	→		*ARR1*	7.62E-11	
B9-155	PhOCP	→	3PhOC + NO2	*ARR2*	5.20E+16	13850.00
B9-156	PhOCP + HO	→		*ARR1*	2.69E-11	
B9-157	PhOCG + HO	→		*ARR1*	3.19E-11	
B9-158	PhOCA + HO	→		*ARR1*	3.53E-11	
B9-159	PhON + HO	→		*ARR1*	2.16E-11	
B9-160	PhOH + HO	→		*ARR1*	3.54E-11	
B9-161	PhOO + HO	→		*ARR1*	4.15E-11	
B9-162	PhOD + HO	→		*ARR1*	3.75E-11	
B9-163	PhOD + NO3	→		*ARR1*	2.74E-13	
B9-164	ONaONBp + HO	→		*ARR1*	1.17E-10	
B9-165	ONaONBp + NO3	→		*ARR1*	1.91E-13	
B9-166	ONaOHBp + HO	→		*ARR1*	1.36E-10	

B9-167	ONaOHBp + NO3	→	*ARR1*	1.91E-13		
B9-168	ONaOOBp + HO	→	*ARR1*	3.31E-10		
B9-169	ONaOOBp + NO3	→	*ARR1*	2.08E-13		
B9-170	ONaOKBp + HO	→	*ARR1*	3.54E-11		
B9-171	ONaOKBp + NO3	→	*ARR1*	1.89E-13		
B9-172	OPhDD + HO	→	*ARR1*	2.43E-11		
B9-173	ONaONpar + HO	→	*ARR1*	3.61E-10		
B9-174	ONaOHpar + O3	→	*ARR1*	1.15E-17		
B9-175	ONaONpar + NO3	→	*ARR1*	3.05E-13		
B9-176	ONaOHpar + HO	→	*ARR1*	4.19E-10		
B9-177	ONaOHpar + O3	→	*ARR1*	2.62E-16		
B9-178	ONaOHpar + NO3	→	*ARR1*	3.05E-13		
B9-179	ONaOOpar + HO	→	*ARR1*	1.16E-09		
B9-180	ONaOOpar + O3	→	*ARR1*	3.67E-16		
B9-181	ONaOOpar + NO3	→	*ARR1*	2.73E-13		
B9-182	ONaOKpar + O3	→	*ARR1*	5.24E-18		
B9-183	ONaOKpar + NO3	→	*ARR1*	7.96E-15		
B9-184	ONaQuin + HO	→	*ARR1*	3.49E-11		
B9-185	ONaNOOK + HO	→	*ARR1*	3.23E-11		
B9-186	ONaNOOK + NO3	→	*ARR1*	5.30E-15		
B9-187	ONaHOOK + HO	→	*ARR1*	6.11E-11		
B9-188	ONaHOOK + NO3	→	*ARR1*	5.30E-15		
B9-189	ONaOOOK + HO	→	*ARR1*	7.35E-11		
B9-190	ONaOOOK + NO3	→	*ARR1*	9.95E-15		
B9-191	ONaOOKK + HO	→	*ARR1*	3.55E-11		
B9-192	ONaOOKK + NO3	→	*ARR1*	2.02E-15		
B9-193	OPhODKD + HO	→	*ARR1*	3.56E-11		
B9-194	OPhODKD + NO3	→	*ARR1*	2.87E-13		
B9-195	ONaONort + HO	→	*ARR1*	3.40E-10		
B9-196	ONaONort + O3	→	*ARR1*	8.24E-18		
B9-197	ONaONort + NO3	→	*ARR1*	3.43E-13		
B9-198	ONaOHort + HO	→	*ARR1*	4.75E-10		
B9-199	ONaOHort + O3	→	*ARR1*	1.87E-16		
B9-200	ONaOHort + NO3	→	*ARR1*	3.43E-13		
B9-201	ONaOOort + HO	→	*ARR1*	5.14E-10		
B9-202	ONaOOort + O3	→	*ARR1*	2.62E-16		
B9-203	ONaOOort + NO3	→	*ARR1*	3.09E-13		
B9-204	ONaOKort + HO	→	*ARR1*	3.55E-10		
B9-205	ONaOKort + O3	→	*ARR1*	3.74E-18		
B9-206	ONaOKort + NO3	→	*ARR1*	8.03E-15		
B9-207	OPhDCD + HO	→	*ARR1*	4.90E-11		
B9-208	OPhDCA + HO	→	*ARR1*	2.83E-11		
B9-209	OPhDNOD + HO	→	*ARR1*	6.00E-11		
B9-210	OPhDNOD + NO3	→	*ARR1*	4.66E-14		
B9-211	OPhDHOD + HO	→	*ARR1*	7.09E-11		
B9-212	OPhDHOD + NO3	→	*ARR1*	4.55E-13		
B9-213	OPhDOOD + HO	→	*ARR1*	8.45E-11		
B9-214	OPhDOOD + NO3	→	*ARR1*	4.58E-13		
B9-215	OPhDKOD + HO	→	*ARR1*	7.20E-11		
B9-216	OPhDKOD + NO3	→	*ARR1*	1.34E-14		
B9-217	OPhUAnhy + HO	→	*ARR2*	0.622E-11	-540.0	
B9-218	OPhUAnhy + NO3	→	*ARR1*	0.272E-14		
B9-219	OPhAUA + HO	→	*ARR1*	5.23E-11		
B9-220	OPhAUA + NO3	→	*ARR1*	3.40E-13		
B9-221	OPhAD + HO	→	*ARR1*	1.38E-11		
B9-222	OPhD + HO	→	*ARR1*	1.46E-11		
B9-223	OHPhUA + HO	→	*ARR1*	6.18E-11		
B9-224	OOPhUA + HO	→	*ARR1*	1.01E-10		
B9-225	VOOPhUA + HO	→	*ARR1*	7.00E-11		
B9-226	NaOONBp + HO	→	*ARR1*	8.11E-11		
B9-227	NaOONBp + NO3	→	*ARR1*	9.09E-13		
B9-228	NaOOHBp + HO	→	*ARR1*	9.41E-11		
B9-229	NaOOHBp + NO3	→	*ARR1*	9.09E-13		
B9-230	NaOOOBp + HO	→	*ARR1*	2.16E-10		
B9-231	NaOOOBp + NO3	→	*ARR1*	9.26E-13		
B9-232	NaOOKBp + HO	→	*ARR1*	2.64E-11		
B9-233	NaOOKBp + NO3	→	*ARR1*	9.07E-13		
B9-234	NaOONort + HO	→	*ARR1*	9.16E-11		

B9-235	NaOONort + O3	→		*ARR1*	8.24E-18	
B9-236	NaOONort + NO3	→		*ARR1*	3.43E-13	
B9-237	NaOOHort + HO	→		*ARR1*	2.26E-10	
B9-238	NaOOHort + O3	→		*ARR1*	1.87E-16	
B9-239	NaOOHort + NO3	→		*ARR1*	3.43E-13	
B9-240	NaOOOort + HO	→		*ARR1*	2.65E-10	
B9-241	NaOOOort + O3	→		*ARR1*	2.62E-16	
B9-242	NaOOOort + NO3	→		*ARR1*	3.09E-13	
B9-243	NaOOKort + HO	→		*ARR1*	1.06E-10	
B9-244	NaOOKort + O3	→		*ARR1*	3.74E-18	
B9-245	NaOOKort + NO3	→		*ARR1*	8.03E-15	
B9-246	PhDOOND + HO	→		*ARR1*	3.00E-11	
B9-247	PhDOOND + NO3	→		*ARR1*	4.98E-14	
B9-248	PhDOOKD + HO	→		*ARR1*	2.96E-11	
B9-249	PhDOOD1 + HO	→		*ARR1*	4.40E-11	
B9-250	PhDOOD1 + NO3	→		*ARR1*	5.68E-13	
B9-251	PhOOAnhy + HO	→		*ARR1*	1.22E-11	
B9-252	PhA + HO	→		*ARR1*	5.77E-12	
B9-253	PhDKND + HO	→		*ARR1*	2.52E-11	
B9-254	PhDKND + NO3	→		*ARR1*	2.89E-14	
B9-255	PhDKHD + HO	→		*ARR1*	3.34E-11	
B9-256	PhDKHD + NO3	→		*ARR1*	2.89E-14	
B9-257	PhOUHEst + HO	→		*ARR1*	1.285E-10	
B9-258	PhOUAnhy + HO	→		*ARR2*	4.96E-11	
B9-259	PhOUOEst + HO	→		*ARR1*	1.365E-10	
B9-260	PhPOUA + HO	→		*ARR1*	6.32E-11	
B9-261	PhPOUA	→	3PhOUA + NO2	*ARR2*	5.20E+16	13850.00
B9-262	PhGOUA + HO	→		*ARR1*	6.63E-11	
B9-263	PhAOUA + HO	→		*ARR1*	6.38E-11	
B9-264	PhPOUD + HO	→	HO	*ARR1*	7.02E-11	
B9-265	PhPOUD	→	3PhOUD + NO2	*ARR2*	5.20E+16	13850.00
B9-266	PhGOUD + HO	→		*ARR1*	7.33E-11	
B9-267	PhAOUD + HO	→		*ARR1*	7.07E-11	
B9-268	HPhOUA + HO	→		*ARR1*	7.33E-11	
B9-269	OPhOUA + HO	→		*ARR1*	1.125E-10	
B9-270	VOPhOUA + HO	→		*ARR1*	8.15E-11	
B9-271	PhOUP	→	3PhOU + NO2	*ARR2*	5.20E+16	13850.00
B9-272	PhOUP + HO	→		*ARR1*	5.54E-11	
B9-273	PhOUG + HO	→		*ARR1*	5.85E-11	
B9-274	PhOUA + HO	→		*ARR1*	5.60E-11	
B9-275	NaOKKN + HO	→		*ARR1*	2.89E-12	
B9-276	NaOKKH + HO	→		*ARR1*	1.76E-11	
B9-277	NaOKKK + HO	→		*ARR1*	3.53E-12	
B9-278	NaNKON + HO	→		*ARR1*	2.65E-12	
B9-279	NaHKON + HO	→		*ARR1*	1.12E-11	
B9-280	NaOKON + HO	→		*ARR1*	1.41E-11	
B9-281	NaKKON + HO	→		*ARR1*	4.76E-12	
B9-282	PhGND + HO	→		*ARR1*	2.85E-11	
B9-283	PhGND + NO3	→		*ARR1*	1.89E-14	
B9-284	PhAND + HO	→		*ARR1*	2.60E-11	
B9-285	PhAND + NO3	→		*ARR1*	1.89E-14	
B9-286	PhPND + HO	→		*ARR1*	2.55E-11	
B9-287	PhPND	→	3PhND + NO2	*ARR2*	5.20E+16	13850.00
B9-288	PhPND + NO3	→		*ARR1*	1.89E-14	
B9-289	PhNA + HO	→		*ARR1*	5.86E-12	
B9-290	PhNG + HO	→		*ARR1*	8.56E-12	
B9-291	PhNP	→	3PhN + NO2	*ARR2*	5.20E+16	13850.00
B9-292	PhNP + HO	→		*ARR1*	5.24E-12	
B9-293	PhAnhy + HO	→		*ARR1*	8.44E-13	
B9-294	PhEstH + HO	→	0.55 PhAnhy	*ARR1*	1.01E-11	
B9-295	PhEstO + HO	→	0.28 PhAnhy	*ARR1*	1.59E-11	
B9-296	PhGA + HO	→		*ARR1*	1.61E-11	
B9-297	PhPA + HO	→		*ARR1*	1.30E-11	
B9-298	PhAA + HO	→	0.1 3PhA	*ARR1*	1.36E-11	
B9-299	PhPA	→	3PhA + NO2	*ARR2*	5.20E+16	13850.00
B9-300	HPhA + HO	→	0.23 3PhA	*ARR1*	1.64E-11	
B9-301	OPhA + HO	→	0.1 1PhA	*ARR1*	3.44E-11	
B9-302	VOPhA + HO	→		*ARR1*	4.93E-12	

B9-303	PhGD + HO	→	0.20 3PhD	*ARR1*	1.64E-11	
B9-304	PhPD	→	3PhD + NO2	*ARR2*	5.20E+16	13850.00
B9-305	PhPD + HO	→		*ARR1*	1.64E-11	
B9-306	HPhD + HO	→	0.23 3PhD	*ARR1*	1.64E-11	
B9-307	VOPhD + HO	→		*ARR1*	9.40E-12	
B9-308	NaOOO + HO	→		*ARR1*	4.955E-10	
B9-309	NaVOO + HO	→		*ARR1*	1.00E-10	
B9-310	NaHO + HO	→		*ARR1*	7.80E-11	
B9-311	NaOOK + HO	→		*ARR1*	7.51E-11	
B9-312	NaOOK + O3	→		*ARR1*	8.39E-17	
B9-313	NaOOK + NO3	→		*ARR1*	3.09E-13	
B9-314	NaOOONBp + HO	→		*ARR1*	2.06E-10	
B9-315	NaOOONBp + NO3	→		*ARR1*	9.08E-13	
B9-316	NaOOOHBp + HO	→		*ARR1*	2.17E-10	
B9-317	NaOOOHBp + NO3	→		*ARR1*	4.45E-12	
B9-318	NaOOOOBp + HO	→		*ARR1*	2.06E-10	
B9-319	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	7.213	0
75	GLYA	0.002	0
91	GLYG	0	0
107	PhD	0.149	0
123	PhA	0.01	0
123	OPhD	0.007	0
129	NAPH	20.078	0
135	PhDD	9.987	0.003
135	PhKD	0.015	0
137	PhOD	0	0
139	HPhD	0	0
139	OPhA	0	0
145	NaO	1.559	0
149	PhAnhy	1.091	0.125
149	PhUA	0	0
149	PhDCD	0.006	0
151	PhEstO	0	0
151	OPhDD	0.07	0.007
151	PhAD	0.427	0.019
153	PhOA	0	0
153	PhHD	0	0
155	HPhA	0	0
159	NaKK	0.325	0
159	NaQuin	0.804	0
161	ONaO	0.114	0.007
161	NaH	0	0
161	NaOPEN	3.101	0.036
161	NaOKort	0.652	0.001
161	NaOKpar	1.224	0.004
161	NaOO	0.093	0.006
163	NaOOpar	0	0
163	NaOOort	0	0
163	PhKDD	0.12	0
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	PhKG	0	0
167	OPhAD	0.001	0.002
167	PhEstH	0	0
167	PhAA	0.006	0.011
168	VOPhD	0.725	0.067
169	PhOG	0	0
174	NaV	2.863	0.001
175	ONaQuin	0.005	0
175	NaKKEpox	2.252	0.001
175	PhUAnhy	0.21	0.172
177	NaOPENEpox	0.862	0.001
177	NaOOO	0.017	0.027
177	NaHO	0	0
177	NaOOK	0.069	0.02
177	ONaOPEN	0.058	0.096
177	PhKAnhy	0.011	0.014
177	NaOPENOL	0.154	0.164
177	ONaOKpar	0.014	0.008
177	NaOOKort	0	0
177	ONaOKort	0	0
177	NaOKEpox	0.022	0
177	PhUOEst1	0	0
177	PhAUD1	0	0
177	PhUOEst2	0	0
177	PhAUD2	0	0
179	PhDKA	0.004	0.004
179	NaOHpar	0	0
179	ONaOOort	0	0
179	NaOOOort	0	0
179	PhAKD	0.007	0.008
179	NaOHort	0	0
179	NaOOEpox	0	0
179	ONaOOpar	0	0
179	PhOAnhy	0.04	0.001
181	OPhDCA	0	0
181	PhOUG	0	0
181	PhOOEst	0	0
181	PhDOOD1	0.017	0

m/z	species	Gas	Part.
181	**HPhUA**	0	0
181	**PhDHD**	0	0
181	**PhKOA**	0	0
181	**PhEpoxG**	0	0
181	**OOPhUA**	0	0
181	**PhAOD**	0	0
181	**OPhOUA**	0	0
181	**OPhEpoxA**	0	0
182	**PhND**	0.002	0
183	**PhGA**	0	0
184	**VOPhA**	0.167	0.306
190	**NaVO**	0.502	0.036
191	**NaOKKK**	0	0
191	**PhKDKD**	0.041	0.005
191	**PhDKKD**	0.194	0.025
191	**PhEpoxAnhy**	0.074	0.043
191	**OPhUAnhy**	0.004	0.01
191	**PhOUAnhy**	0.009	0.022
193	**OPhDEpoxD**	0.005	0.001
193	**PhOUOEst**	0	0
193	**PhGUD1**	0	0
193	**PhGUD2**	0	0
193	**PhEpoxOEst**	0	0
193	**PhODKD**	0.314	0.401
193	**PhAOUD**	0	0
193	**PhUHEst1**	0	0
193	**PhUHEst2**	0	0
193	**PhAEpoxD**	0.052	0.04
193	**PhDKOD**	0.564	0.644
193	**NaOOKK**	0	0
193	**PhAUA**	0.001	0.002
195	**PhAKA**	0	0
195	**PhOOAnhy**	0.002	0.003
195	**ONaOHort**	0	0
195	**NaOOHort**	0	0
195	**NaOHEpox**	0	0
195	**PhDOOD**	0	0
195	**ONaOHpar**	0	0
195	**NaOOOK**	0	0
197	**HPhOUA**	0	0
197	**OHPhUA**	0	0
197	**PhOHEst**	0	0
197	**PhGOD**	0	0

m/z	species	Gas	Part.
197	**PhKOG**	0	0
197	**PhAOA**	0	0
197	**PhAHD**	0	0
197	**HPhEpoxA**	0	0
197	**OPhKOA**	0	0
198	**PhNA**	0	0
205	**PhKKAnhy**	0.009	0.014
206	**NaVOO**	0.017	0.032
207	**PhKOAnhy**	0.038	0.077
207	**PhOKAnhy**	0.013	0.027
208	**NaONpar**	0.122	0.01
208	**NaONort**	0.519	0.043
209	**PhOUHEst**	0	0
209	**PhGOUD**	0	0
209	**NaOKKH**	0	0
209	**OPhODKD**	0.291	0.587
209	**PhOKOEst**	0	0
209	**PhKOOEst**	0	0
209	**PhDOOKD**	0	0
209	**PhEpoxHEst**	0	0
209	**OPhDKOD**	0	0
209	**ONaOOKK**	0	0
209	**PhAOKD**	0	0
209	**PhDKHD**	0	0
209	**PhGUA1**	0	0
209	**PhGUA2**	0	0
209	**PhGEpoxD**	0	0
209	**OPhAUA**	0	0
209	**PhAOUA**	0	0
209	**PhAKOD**	0	0
209	**PhAEpoxA**	0	0
210	**PhUP**	0.141	0
210	**VOPhUA**	0.021	0.047
210	**PhDND**	0.002	0
211	**PhDOOOD**	0	0
211	**OPhDOOD**	0	0
211	**PhDHOD**	0.001	0.001
211	**ONaOOOK**	0	0
211	**NaHOOK**	0	0.001
212	**PhPD**	3.863	0.004
213	**PhAOOA**	0	0
213	**PhGOA**	0	0
213	**HPhKOA**	0	0

m/z	species	Gas	Part.
214	**PhNG**	0	0
214	**PhOP**	0.037	0.001
223	**PhKAKA**	0	0
224	**ONaONpar**	0.001	0.002
224	**ONaONort**	0.004	0.006
224	**NaOONort**	0.048	0.081
224	**NaONEpox**	0.332	0.026
225	**PhGOUA**	0	0
225	**PhOKHEst**	0	0
225	**PhGOKD**	0	0
225	**PhKOHEst**	0	0
225	**NaOKBp**	0	0
225	**PhAOKA**	0	0
225	**PhAKOA**	0	0.001
225	**PhGKOD**	0	0
225	**PhAEpoxG**	0	0
226	**VOPhOUA**	0	0.012
226	**PhOUP**	0.003	0.001
226	**VOOPhUA**	0	0.005
226	**PhEpoxP**	0.03	0
226	**VOPhEpoxA**	0.009	0.016
226	**PhAND**	0.001	0.002
227	**PhDOOHD**	0	0
227	**NaOOBp**	0	0
227	**OPhDHOD**	0	0
227	**ONaHOOK**	0	0
228	**PhPA**	0.947	0.597
238	**NaOKKN**	0.018	0.026
238	**NaKKON**	0	0
238	**PhNDKD**	0	0
238	**PhPUD1**	0.331	0.023
238	**PhPUD2**	0.252	0.012
238	**PhDKND**	0.005	0.005
240	**NaOKON**	0	0
240	**PhDNOD**	0.521	1.052
240	**NaNOOK**	0.206	0.386
241	**PhGOKA**	0	0
241	**PhGKOA**	0	0
241	**ONaOKBp**	0	0
241	**NaOOKBp**	0.697	0.024
242	**VOPhKOA**	0.001	0.034
242	**PhPOD**	0.026	0.022
242	**PhKOP**	0.01	0.005

m/z	species	Gas	Part.
242	**PhGND**	0	0
243	**NaOHBp**	0	0
243	**ONaOOBp**	0	0
243	**NaOOOBp**	0	0
254	**PhPOUD**	0.015	0.027
254	**PhPUA1**	0.111	0.194
254	**PhPUA2**	0.08	0.14
254	**PhPEpoxD**	0.168	0.004
256	**NaHKON**	0	0
256	**OPhDNOD**	0.005	0.014
256	**PhDOOND**	0.002	0.005
256	**ONaNOOK**	0.001	0.003
258	**PhPOA**	0.015	0.027
259	**PhNP**	0	0
259	**ONaOHBp**	0	0
259	**NaOOHBp**	0	0
259	**NaOOOOBp**	0	0
270	**PhPOUA**	0.014	0.048
270	**PhPOKD**	0.021	0.036
270	**PhPKOD**	0.06	0.103
270	**PhAEpoxP**	0.065	0.099
272	**NaONBp**	0.131	0.002
275	**NaOOOHBp**	0	0
285	**NaNKON**	0	0
286	**PhPOKA**	0.01	0.07
286	**PhPKOA**	0.021	0.216
287	**PhPND**	0	0
288	**ONaONBp**	0.001	0.001
288	**NaOONBp**	0.014	0.012
304	**NaOOONBp**	0	0