Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Materials

The SOA Formation Model Combined with Semiempirical Quantum Chemistry to Predict UV-Vis Absorption of Secondary Organic Aerosols

Min Zhong[a], Myoseon Jang*[a] Alexander Oliferenko[b] and Alan R. Katritzky[b]

[a] *Department of Environmental Engineering Sciences, University of Florida, Gainesville, 32611, Florida, USA*

[b] *Center for Heterocyclic Compounds, Department of Chemistry, University of Florida, Gainesville, Florida 32611, USA;*

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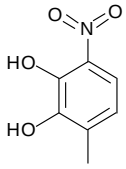
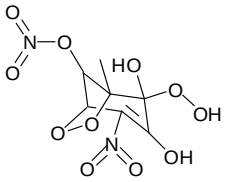
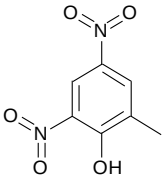
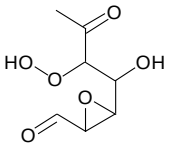
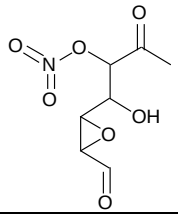
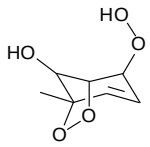
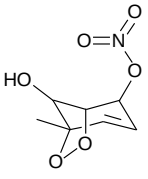
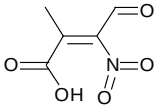
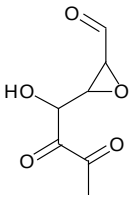
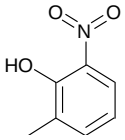
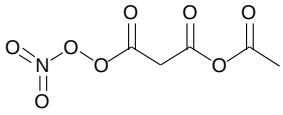
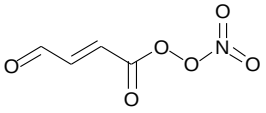
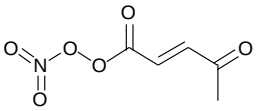
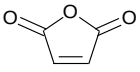
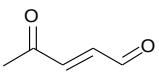
Table S1. Chemical structure of toluene SOA products

MCM name[a]	IUPAC name	Structure
MNCATECH	3-methyl-6-nitrobenzene-1,2-diol	
MNNCATCOOH	(2R)-2-hydroperoxy-2,3-dihydroxy-1-methyl-4-nitro-6,7-dioxabicyclo[3.2.1]oct-3-en-8-yl nitrate	
DNCRES	2-methyl-4,6-dinitro-phenol	
TLEMUCOOH	3-(2-hydroperoxy-1-hydroxy-3-oxo-butyl)-oxirane-2-carbaldehyde	
TLEMUCNO3	1-(3-formyloxiran-2-yl)-1-hydroxy-3-oxobutan-2-yl nitrate	
TLBIPEROOH	(1S,4S,5S)-4-hydroperoxy-1-methyl-6,7-dioxabicyclo[3.2.1]oct-2-en-8-ol	
TLBIPERNO3	(1S,2S,5S)-8-hydroxy-5-methyl-6,7-dioxabicyclo[3.2.1]oct-3-en-2-yl nitrate	

NC4MDCO2H	(Z)-2-methyl-3-nitro-4-oxobut-2-enoic acid	
TLEMUCCO	3-(1-hydroxy-2,3-dioxobutyl)oxirane-2-carbaldehyde	
TOL1OHNO2	2-methyl-6-nitrophenol	
ACCOMEPAN	3-acetoxy-3-oxopropanoic nitric peroxyanhydride	
MALDIALPAN	nitric (E)-4-oxobut-2-enoic peroxyanhydride	
C5COO2NO2	nitric (E)-4-oxopent-2-enoic peroxyanhydride	
MALANHY	furan-2,5-dione	
C5DICARB	4-Oxo-pent-2-enal	

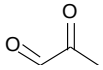
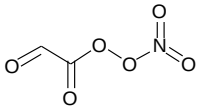
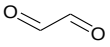
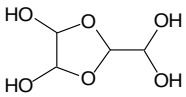
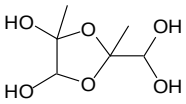
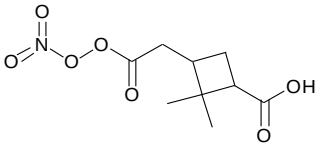
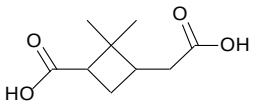
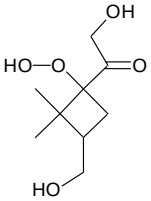
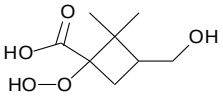
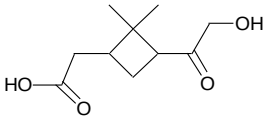
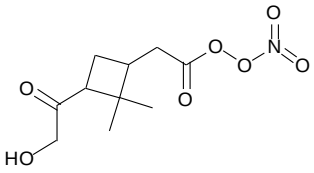
MGLYOX	2-oxopropanal	
GLYPAN	nitric 2-oxoacetic peroxyanhydride	
GLYOX	oxalaldehyde	
GLYOX oligomer	2-Dihydroxymethyl-[1,3]dioxolane-4,5-diol	
MGLYOX oligomer	2-Dihydroxymethyl-2,4-dimethyl-[1,3]dioxolane-4,5-diol	

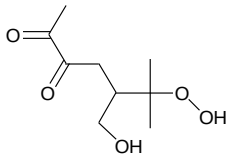
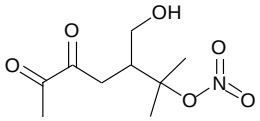
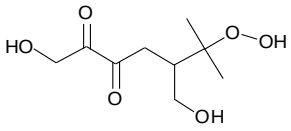
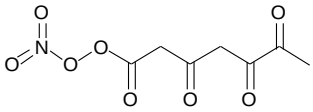
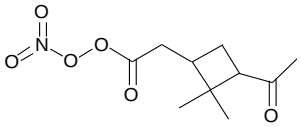
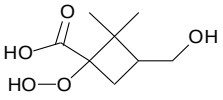
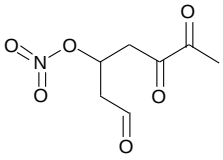
Table S2. Representative products of toluene SOA and their mass percentages at different NO_x conditions

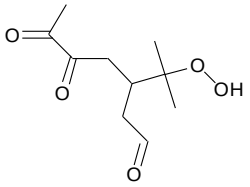
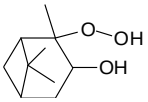
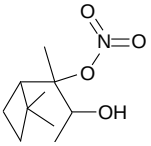
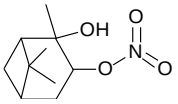
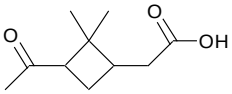
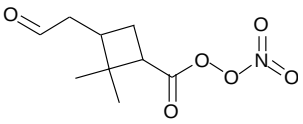
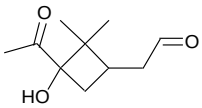
Group (*i*, *j*)	***k***	**Products name**[a]	***MW*$_k$**	**λ_{max}**[b] **(nm)**	***f***[b]	***F*$_k$**[c] **(%)**		
						H NO_x (T1)	M NO_x (T2)	L NO_x (T3)
1, PO	1	MNCATECH	169	330, 228	0.05, 0.40	26.27	30.48	26.14
	2	MNNCATCOOH	281	270, 199, 189, 188	0.3, 0.15, 0.31, 0.03	2.95	6.36	6.47
	3	DNCRES	191	321, 229, 227, 222, 203	0.04, 0.17, 0.40, 0.82, 0.08	2.00	0.88	0.32
1, H-m	4	TLEMUCOOH	190	177, 165, 161	0.04, 0.05, 0.03	1.04	3.04	4.41
	5	TLEMUCNO3	190	177, 165, 161	0.04, 0.05, 0.03	2.40	1.57	1.10
2, PO	6	TLBIPEROOH	174	216, 213, 163, 153, 143	0.19, 0.11, 0.13, 0.10, 0.05	2.13	8.68	14.00
	7	TLBIPERNO3	174	415, 233	0.06, 0.07	3.85	3.46	2.78
2, H-s	8	NC4MDCO2H	159	228, 226, 221, 202, 177, 172, 168	0.15, 0.08, 0.21, 0.26, 0.22, 0.19, 0.05	6.71	3.19	1.38
2, H-f	9	TLEMUCCO	156	202, 148	0.35, 0.03	0.53	0.81	1.09
3, PO	10	TOL1OHNO2	153	316, 222	0.04, 0.17	0.77	0.51	0.23
3, H-f	11	ACCOMEPAN	207	206, 187, 174	0.08, 0.26, 0.25	2.29	10.34	7.67
4, H-m	12	MALDIALPAN	161	208, 190, 176, 158	0.07, 0.27, 0.26, 0.05	0.59	0.48	0.41
	13	C5COO2NO2	175	227, 184, 176	0.59, 0.22, 0.26	0.99	1.03	1.17
5, H-m	14	MALANHY	98	230	0.17	2.26	1.00	1.01
	15	C5DICARB	98	223, 166, 162, 155	0.65, 0.06, 0.09, 0.42	0.55	0.21	0.14
	16	MGLYOX (oligomer)	72	193, 171, 160, 155	0.20, 0.34	4.98	2.55	2.16
	17	GLYPAN	135	213, 189, 183, 168	0.13, 0.04, 0.47, 0.53	1.12	0.53	0.33
5, H-f	18	GLYOX (oligomer)	58	196, 182, 163, 160	0.14, 0.06, 0.39, 0.11	37.17	23.26	27.30

a: The names of chemicals are from MCM mechanism; b: λ_{max} and *f* are calculated using NDDO based AM1 semiempirical quantum chemistry method; c: F_k is the mass percentage of the *k*th species, obtained by the mass balance of chemical compounds in toluene SOA.

Table S3.Chemical structure of α-pinene SOA from MCM mechnism

MCM name	IUPAC name	Structure
C811PAN	2,2-dimethyl-3-(2-(nitroperoxy)-2-oxoethyl)cyclobutanecarboxylic acid	
PINIC	3-(carboxymethyl)-2,2-dimethylcyclobutanecarboxylic acid	
C921OOH	1-(1-hydroperoxy-3-(hydroxymethyl)-2,2-dimethylcyclobutyl)-2-hydroxyethanone	
C812OOH	1-hydroperoxy-3-(hydroxymethyl)-2,2-dimethylcyclobutanecarboxylic acid	
HOPINONIC	2-(3-(2-hydroxyacetyl)-2,2-dimethylcyclobutyl)acetic acid	
C920PAN	2-(3-(2-hydroxyacetyl)-2,2-dimethylcyclobutyl)acetic nitric peroxyanhydride	

C98OOH	6-hydroperoxy-5-(hydroxymethyl)-6-methylheptane-2,3-dione	
C98NO3	3-(hydroxymethyl)-2-methyl-5,6-dioxoheptan-2-yl nitrate	
C922OOH	6-hydroperoxy-1-hydroxy-5-(hydroxymethyl)-6-methylheptane-2,3-dione	
C7PAN3	nitric 3,5,6-trioxoheptanoic peroxyanhydride	
C10PAN2	2-(3-acetyl-2,2-dimethylcyclobutyl)acetic nitric peroxyanhydride	
C97OOH	1-(1-hydroperoxy-3-(hydroxymethyl)-2,2-dimethylcyclobutyl)ethanone	
C717NO3	1,5,6-trioxoheptan-3-yl nitrate	

C108OOH	3-(2-hydroperoxypropan-2-yl)-5,6-dioxoheptanal	
APINAOOH	2-hydroperoxy-2,6,6-trimethylbicyclo[3.1.1]heptan-3-ol	
APINANO3	3-hydroxy-2,6,6-trimethylbicyclo[3.1.1]heptan-2-yl nitrate	
APINBNO3	2-hydroxy-2,6,6-trimethylbicyclo[3.1.1]heptan-3-yl nitrate	
PINONIC	2-(3-acetyl-2,2-dimethylcyclobutyl)acetic acid	
C89PAN	2,2-dimethyl-3-(2-oxoethyl)cyclobutanecarboxylic nitric peroxyanhydride	
C107OH	2-(3-acetyl-3-hydroxy-2,2-dimethylcyclobutyl)acetaldehyde	

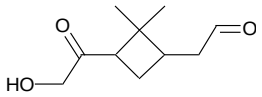
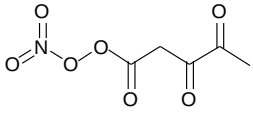
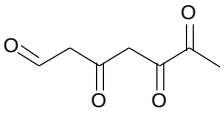
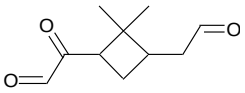
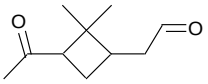
C109OH	2-(3-(2-hydroxyacetyl)-2,2-dimethylcyclobutyl)acetaldehyde	
C5PAN9	nitric 3,4-dioxopentanoic peroxyanhydride	
CO235C6CHO	3,5,6-trioxoheptanal	
C109CO	2-(2,2-dimethyl-3-(2-oxoethyl)cyclobutyl)-2-oxoacetaldehyde	
PINAL	2-(3-acetyl-2,2-dimethylcyclobutyl) acetaldehyde	

Table S4. Representative products of α-pinene SOA and their mass percentages in SOA at different NO_x conditions

Group (*i*, *j*)	***k***	**Products name**[a]	***MW*$_k$**	**λ_{max}**[b] **(nm)**	***f***[b]	***F*$_k$**[c] **(%)**	
						H NO_x (A1)	L NO_x (A2)
1, H-s	1	C811PAN	247	183, 161	0.27, 0.11	4.59	3.98
	2	PINIC	186	181, 174, 164, 141, 135	0.25, 0.06, 0.03, 0.05, 0.09	0.02	1.98
	3	C921OOH	204	192, 186, 178, 167, 160, 156	0.09, 0.12,0.09, 0.08, 0.06, 0.07	0.09	1.30
	4	C812OOH	190	187, 186, 169, 164, 157	0.14, 0.10, 0.09, 0.05, 0.11	0.04	0.92
	5	HOPINONIC	200	176, 171, 169, 162, 139	0.25, 0.22, 0.12, 0.03, 0.07	0.04	1.19
1, H-m	6	C920PAN	261	196, 182, 171	0.07, 0.03, 0.06	8.40	3.91
	7	C98OOH	204	201, 167	0.29, 0.14	2.72	10.43
	8	C98NO3	233	188, 183	0.18, 0.03	6.46	2.62
	9	C922OOH	220	204, 177	0.32, 0.17	0.09	1.34
1, H-f	10	C7PAN3	233	205, 192	0.08, 0.35	18.43	3.54
2, H-s	11	C10PAN2	245	187, 171, 167	0.04, 0.08, 0.04	16.30	5.97
	12	C97OOH	188	197, 186, 180, 157, 142, 135	0.05, 0.05, 0.23, 0.05, 0.06, 0.09	0.49	6.13
2, H-f	13	C717NO3	203	184, 182, 177, 174, 165, 155	0.08, 0.19, 0.05, 0.06, 0.09, 0.06	5.28	3.12
	14	C108OOH	216	202	0.26	4.39	14.88
3, PO	15	APINAOOH	186	160, 158, 156, 153, 139, 137	0.16, 0.13, 0.07, 0.17, 0.09, 0.10	0.07	2.32
	16	APINANO3	215	174, 162, 151, 147, 146	0.07, 0.06, 0.2, 0.06, 0.08	0.93	2.42
	17	APINBNO3	215	202, 168, 158, 153	0.05, 0.04, 0.06, 0.22	0.59	1.26
3, H-s	18	PINONIC	184	173, 169, 165, 151	0.31, 0.04, 0.15, 0.08, 0.05	0.09	0.70
3, H-m	19	C89PAN	231	179, 169	0.05, 0.06	3.36	2.14
	20	C107OH	200	182, 175, 162, 145, 141	0.25, 0.06, 0.05, 0.06, 0.14	0.36	3.53
	21	C109OH	200	181, 173, 163, 140, 135	0.25, 0.06, 0.03, 0.05, 0.09	0.28	0.82
	22	C5PAN9	191	199, 184, 174, 168	0.05, 0.22, 0.25, 0.54	2.60	0.60
4, H-f	23	CO235C6CHO	156	159	0.01	2.88	2.85
	24	C109CO	182	200	0.25	0.09	0.42
5, H-m	25	PINAL	168	168, 164, 163, 157, 156, 152	0.03, 0.15, 0.06, 0.14, 0.05, 0.06	20.12	19.46

a: The names of chemicals are from MCM mechanism; b: λ_{max} and *f* are calculated using NDDO based AM1 semiempirical quantum chemistry method; c: F_k is the mass percentage of the *k*th species, obtained by the mass balance of chemical compounds in α-pinene SOA

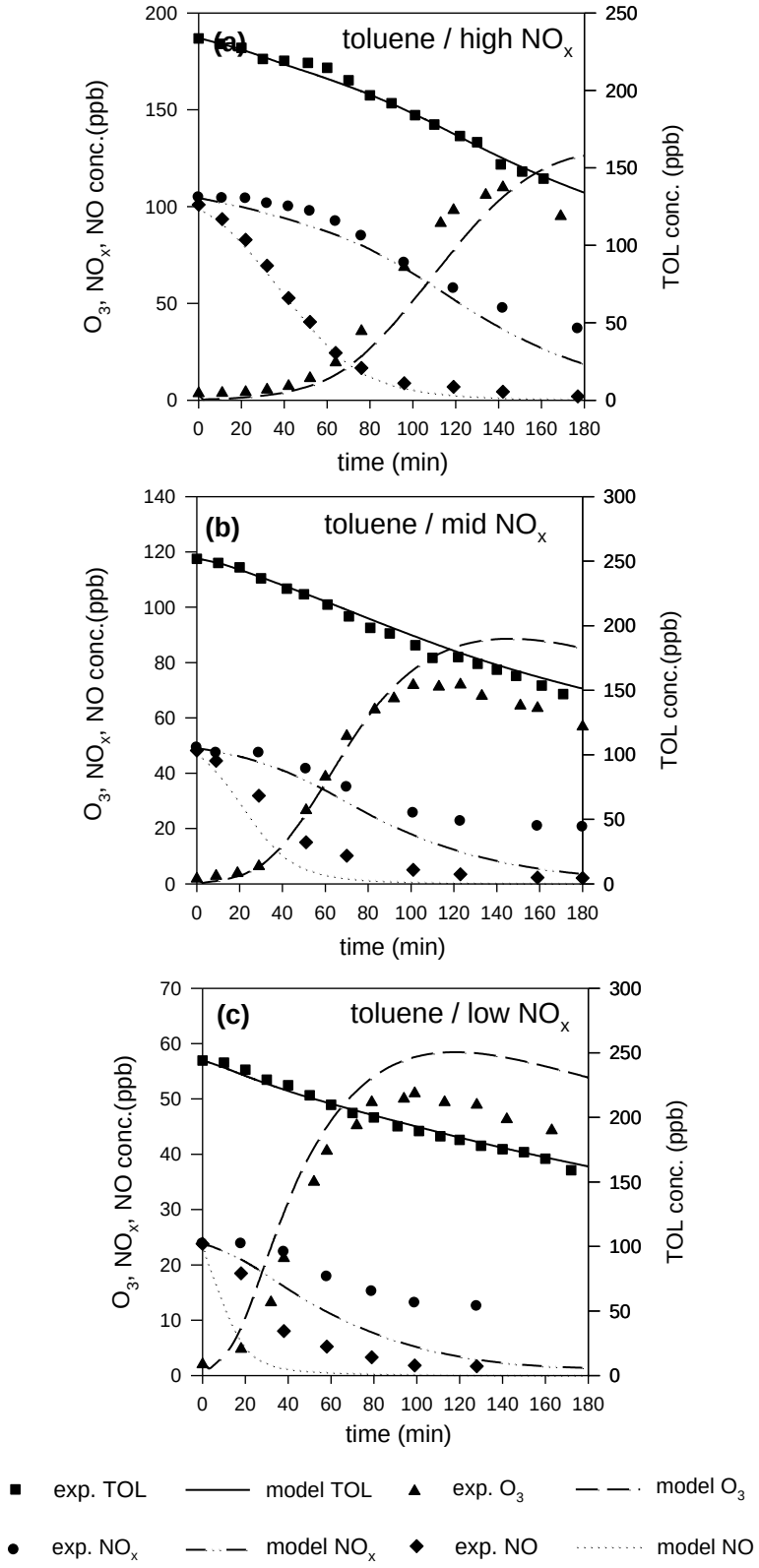


Figure S1: Comparison of model simulated and measured concentrations of toluene, O_3, NO_x, and NO for experiments at high NO_x, mid NO_x and low NO_x levels (T1, T2 and T3)

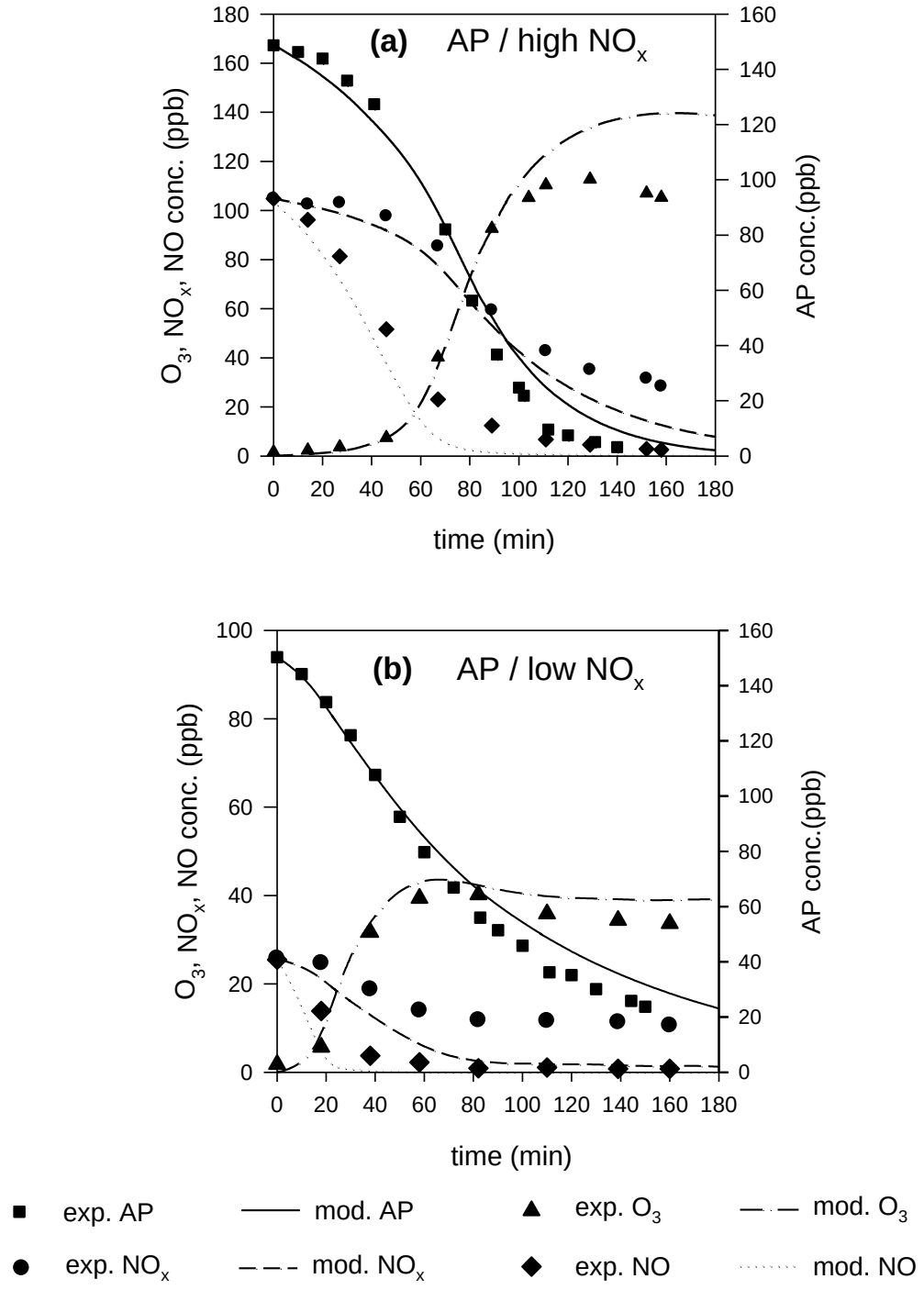


Figure S2: Comparison of model simulated and measured concentrations of α-pinene, O_3, NO_x, and NO for experiments at high NO_x and low NO_x levels (A1and A2)

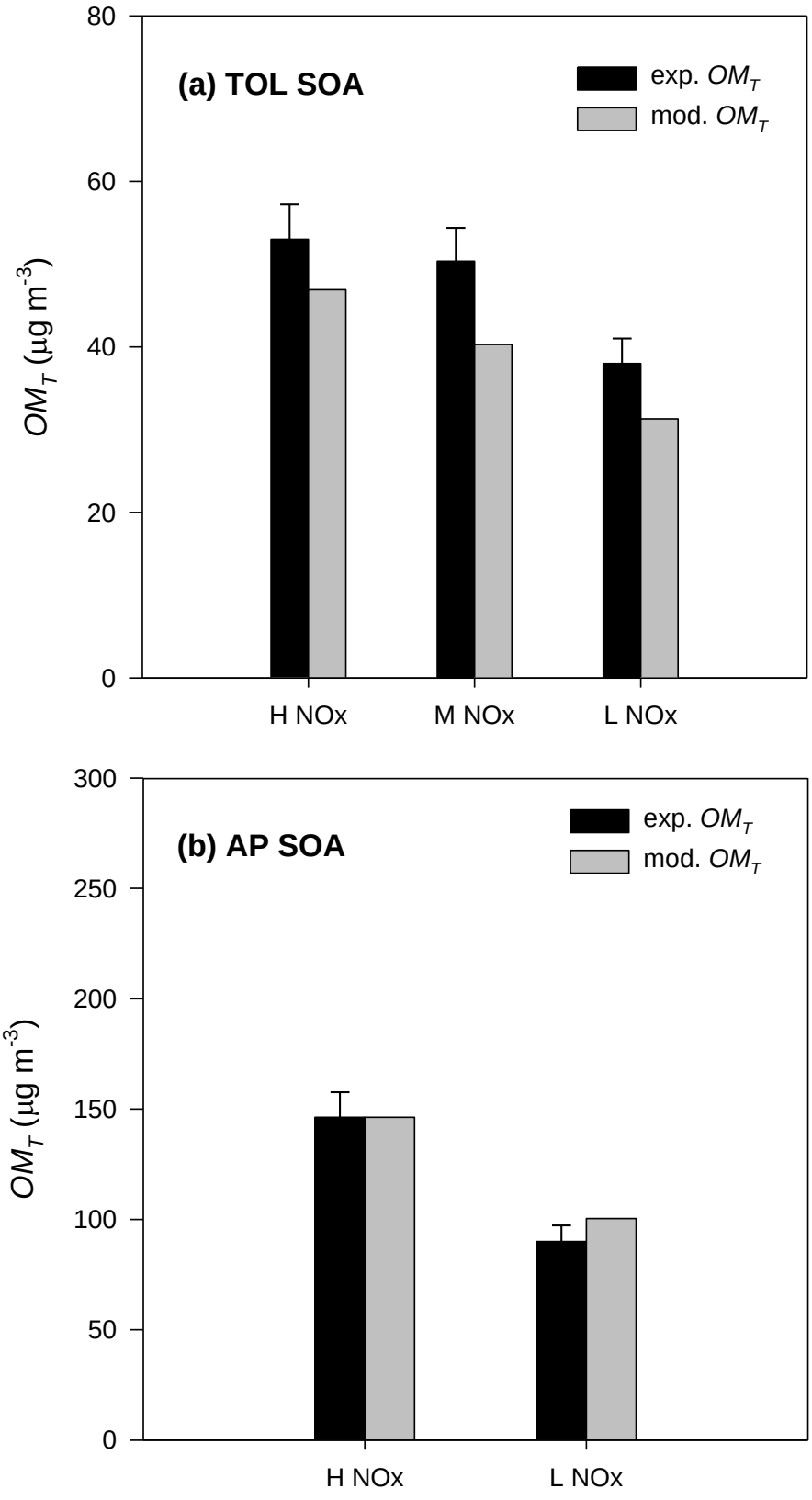


Figure S3: Comparison of the predicted OM_T and the measured OM_T for TOL SOA (a) and AP SOA (b) under different NO_x conditions. T1-T3 for TOL SOA and A1-A2for AP SOA (see Table 1)