Representing Ozone formation from Volatile Chemical Products (VCP) in Carbon Bond (CB) Chemical Mechanisms

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Supplementary Material

Table S-1. The top 39 compounds identified by ranking MIR- and SOA-weighted emissions in the VCPy 2019 US-wide emission inventory. The percentage of emissions, MIR or SOA for each compound is the contribution to that sum over all compounds. The entry for CB6 (Yes or No) indicates whether the compound is considered well-represented by the mechanism species of CB6r5 and CB6r3. C* is the saturation vapor pressure in µg m^{-3}.

Table S-2. Mapping compounds present in VCPy and SPECIATE to the VCP and CB6 mechanism species.

Table S-2. Emissions of CB6 species for the for the Los Angeles box model scenario on July 31, 2011, in moles/day/km^2.

Figure S-1. Meteorological conditions for the Los Angeles box model scenario shown in local standard time for July 29 to August 2, 2011.

Figure S-2. Time series for O_3, NO and NO_2 in the Los Angeles box model scenario shown in local standard time for July 29 to August 2, 2011.

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No.	Name	% Mass	% MIR	% SOA	CB6?	log(C*)
1	Ethanol	17.7	26.5	0.0	Y	8.0
2	Acetone	11.4	8.9	0.0	Y	8.9
3	Isomers of Xylene	1.9	6.5	10.7	Y	7.7
4	Isopropyl Alcohol	7.4	8.8	0.0	N	8.0
5	Toluene	1.9	3.4	10.2	Y	8.1
6	Terpene	0.7	1.6	6.4	Y	7.1
7	2,2,4-Trimethyl-1,3-Pentanediol Isobutyrate (Texanol)	2.1	0.6	5.6	N	4.2
8	Ethylene Glycol	2.9	5.3	0.0	N	5.3
9	Alkanes, C14-16	1.2	0.3	6.1	N	4.6
10	Decamethylcyclopentasiloxane	2.2	0.0	5.0	N	6.6
11	Limonene	0.6	1.4	5.2	Y	7.0
12	C11 Cycloalkanes	1.1	0.4	4.4	Y	6.0
13	C12 Cycloalkanes	0.9	0.3	4.6	Y	5.4
14	Alkyl (C16-C18) Methyl Esters	0.8	0.2	4.7	N	3.9
15	Propylene Glycol	2.0	3.3	0.0	N	5.5
16	Isobutane	3.8	1.1	0.0	N	9.8
17	n-Dodecane	0.9	0.3	2.3	Y	6.2
18	Branched C12 Alkanes	1.3	0.5	1.5	N	6.6
19	Dimethylpolysiloxane	1.0	0.0	2.2	Y	6.8
20	Dimethyl Ether	1.3	1.9	0.0	N	9.8
21	Methanol	1.1	1.9	0.0	Y	8.2
22	Glycerol	1.2	1.8	0.0	N	2.9
23	n-Butane	2.1	0.6	0.0	Y	9.6
24	Ethyl Benzene	0.3	0.9	1.5	Y	7.6
25	Ethylene Glycol Monobutyl Ether	1.1	1.0	0.4	N	6.8
26	1,1-Difluoroethane (HFC-152a)	1.7	0.6	0.0	Y	10.1
27	Methylene Chloride (Dichloromethane)	1.5	0.5	0.0	Y	9.2
28	C13 Branched Alkanes	0.6	0.2	1.1	N	6.2
29	UNC peaks to CBM xylene	0.2	0.6	1.0	Y	7.6
30	Diethylene Glycol Monobutyl Ether	0.5	0.6	0.5	N	5.4
31	Ethyl Cyanoacrylate	0.5	0.7	0.3	N	6.1
32	Methyl Propylcyclohexanes	0.3	0.1	1.0	Y	7.3
33	Cyclotetrasiloxane	0.4	0.0	0.9	N	7.2
34	Formic Acid	0.4	0.9	0.0	Y	8.1

No.	Name	% Mass	% MIR	% SOA	CB6?	log(C*)
35	Isomers Of Undecane	0.4	0.2	0.7	Y	6.5
36	Methyl Ethyl Ketone (2-Butanone)	0.6	0.5	0.0	Y	8.5
37	C10 Cycloalkanes	0.2	0.1	0.7	Y	6.8
38	C13 Cycloalkanes	0.2	0.1	0.8	N	5.4
39	C15 Cycloalkanes	0.1	0.0	0.7	N	2.5

Notes:

The per-mass SOA and MIR values for each compound used to compute % MIR and % SOA may be found in the VCPy database at https://github.com/USEPA/VCPy/tree/main/output/emissions_by_subpuc/2019

Species number 29 “UNC peaks to CBM xylene” is present in the SPECIATE database from VOC speciation profiles that identify compounds as being multiply substituted aromatic (and therefore suitable for mapping to CB model species XYL) without uniquely identifying those compounds. The relevant profiles date from the early 1990s.

Table S-2. Mapping compounds present in VCPy and SPECIATE to the VCP and CB6 mechanism species.

Compound Name	SPECIATE ID	CB6 & VCP Mapping
Ethanol	442	ETOH
Acetone	281	ACET
Isopropyl Alcohol	513	IPOH
Ethylene Glycol	455	EDOH
Isobutane	491	IBTA
Isomers of xylene	507	XYL
Propylene Glycol	680	PDOH
Toluene	717	TOL
Dimethyl Ether	417	DME
Methanol	531	MEOH
Glycerol	471	IVOC
n-Butane	592	4 PAR
1,1-Difluoroethane (HFC-152a)	478	NONR
2,2,4-Trimethyl-1,3-Pentanediol Isobutyrate (Texanol)	115	ESTR + 8 PAR
Methylene Chloride (Dichloromethane)	401	NONR
Propane	671	PRPA
Terpene	705	TERP
Formic Acid	466	FACD
Methyl Ethyl Ketone (2-Butanone)	536	KET + 3 PAR
Branched C12 Alkanes	3198	HPAR
Alkanes, C14-16	3281	IVOC
C11 Cycloalkanes	3227	0.75 HPAR + 2 PAR
n-Undecane	610	0.75 HPAR + 2 PAR
Ethylene Glycol Monobutyl Ether	310	ROH + 2 PAR
C12 Cycloalkanes	3228	HPAR
d-Limonene	392	TERP
n-Dodecane	599	HPAR
n-Heptane	600	0.083 HPAR + 6 PAR
Methyl Acetate	2160	MEAC
Diethylene Glycol Monobutyl Ether	167	ROH + 4 PAR
Ethyl Benzene	449	TOL + PAR
Witch Hazel	774	0.85 NONR + 0.15 ETOH
Ethyl Cyanoacrylate	444	NONR
Alkyl (C16-C18) Methyl Esters	3129	IVOC
Ethyl Acetate	440	ETAC
C13 Branched Alkanes	1934	0.33 IVOC + 0.67 HPAR
Dl-Limonene (Dipentene)	435	TERP
Isomers Of Decane	500	0.5 HPAR + 4 PAR
2-Amino-2-Methyl-1-Propanol	169	NONR

Compound Name	SPECIATE ID	CB6 & VCP Mapping
UNC peaks to CBM xylene	2278	XYL
Diethylene Glycol Monoethyl Ether	331	ROH + 2 PAR
Parachlorobenzotrifluoride	652	NONR
Hydrocarbon Propellant (LPG, Sweetened)	483	PRPA
Sec-Butyl Alcohol	692	ROH
m-Xylene	524	XYL
Isomers Of Undecane	505	0.75 HPAR + 2 PAR
N-Butyl Acetate	593	ESTR + 2 PAR
Methyl Propylcyclohexanes	545	0.5 HPAR + 4 PAR
n-Decane	598	0.5 HPAR + 4 PAR
Branched C11 alkanes	3197	0.75 HPAR + 2 PAR
Propylene Glycol Butyl Ether (1-Butoxy-2-Propanol)	681	ROH + 3 PAR
Styrene	698	XYL
1,1,1,2-Tetrafluoroethane (HFC-134a)	3186	NONR
N-Nonane	603	0.33 HPAR + 5 PAR
Branched C6 Alkanes	3201	6 PAR
Citronella Oil	3121	TERP
C7 Cycloalkanes	550	0.083 HPAR + 6 PAR
Voc Ingredients < 0.1%	772	IVOC
C10 Cycloalkanes	3226	0.5 HPAR + 4 PAR
n-Hexane	601	6 PAR
Ethylmethylcyclohexanes	461	0.33 HPAR + 5 PAR
Other, Misc. VOC Compounds Aggregated In Profile	641	NONR
O-Xylene	620	XYL
C10 Internal Alkenes	316	TERP
Benzyl Alcohol	306	TOL
Isobutyl Alcohol	493	ROH
Isomers Of Butylbenzene	499	TOL + 3 PAR
Diethyl Phthalate	2355	IVOC
Trimethylbenzenes	755	XYL + PAR
C13 Cycloalkanes	3229	0.33 IVOC + 0.67 HPAR
Dipropylene Glycol Monomethyl Ether	395	ROH + 3 PAR
Dipropylene Glycol Methyl Ether Acetate	3165	ETHR + 5 PAR
Diethylene Glycol	406	ROH
Methyl Isobutyl Ketone (Hexone)	539	KET + 5 PAR
Misc. oxygenated compounds	576	IVOC
n-Pentane	605	5 PAR
2-methyldecane	192	0.75 HPAR + 2 PAR
n-Tridecane	609	0.33 IVOC + 0.67 HPAR
n-Butyl Alcohol	595	ROH

Compound Name	SPECIATE ID	CB6 & VCP Mapping
Branched C9 Alkanes	3204	0.33 HPAR + 5 PAR
2,4-Dimethyloctane	151	0.5 HPAR + 4 PAR
Isobutyl Acetate	492	ESTR + 2 PAR
Diacetone	396	KET + 5 PAR
Citrus Terpenes	378	TERP
2,4,5-Trimethylheptane	145	0.33 HPAR + 5 PAR
Branched C7 Alkanes	3202	0.083 HPAR + 6 PAR
Aliphatics	601	0.5 HPAR + 4 PAR
o-Xylene	620	XYL
1,2,4-Trimethylbenzene	30	XYL + PAR
Propylene Glycol Monomethyl Ether (1-Methoxy-2-propanol)	682	ROH
Hexane	601	6 PAR
Linalyl Acetate	9127	TERP
2-Methyloctane	198	0.33 HPAR + 5 PAR
2,2,4,6,6-Pentamethylheptane	114	0.75 HPAR + 2 PAR
Isopropylcyclohexane	515	0.33 HPAR + 5 PAR
Phenoxyethanol	664	TOL + PAR
Butylcyclohexane	312	0.5 HPAR + 4 PAR
Cyclohexane	385	6 PAR
Propylene Glycol N-Propyl Ether	685	ROH + 2 PAR
Acetic Acid	280	AACD
Trimethylcyclohexane	756	0.33 HPAR + 5 PAR
C11 Internal Alkenes	319	IOLE + 7 PAR
Ethyl Methacrylate	3108	OLE + 4 PAR
N,N-Diethyl-M-Toluamide	2202	NONR
2-Methylheptane	193	0.167 HPAR + 6 PAR
Cyclopentane	390	5 PAR
Branched C8 Alkanes	3203	0.167 HPAR + 6 PAR
n-Undecane	610	0.75 HPAR + 2 PAR
m-Xylene	524	XYL
C11 Trialkyl Benzenes	3257	XYL + 3 PAR
2-Methylpentane	2681	6 PAR
2-Methylnonane	197	0.5 HPAR + 4 PAR
Hexyl Acetate	1020	ESTR + 4 PAR
N-Methylpyrrolidinone	85	NONR
Dipropylene Glycol	432	ROH + 2 PAR
2,4-Dimethyl-1-Pentene	146	OLE + 5 PAR
Methyl Amyl Ketone	532	KET + 5 PAR
n-Propyl Alcohol	607	NPOH
Misc. esters	568	ESTR + PAR

Compound Name	SPECIATE ID	CB6 & VCP Mapping
C10 Trialkylbenzenes	3206	XYL + 2 PAR
Propylene Glycol Monomethyl Ether Acetate	684	ETHR + 2 PAR
C15 Cycloalkanes	3231	IVOC
C6 Cycloalkanes	3234	6 PAR
Dimethylnonane	429	0.75 HPAR + 2 PAR
Isoparaffins	3307	0.167 HPAR + 6 PAR
Glycol Ether Dpnb (1-(2-Butoxy-1-Methylethoxy)-2-Propanol)	473	IVOC
1,2,4-Trimethylbenzene	30	XYL + 2 PAR
C8 Cycloalkanes	3258	0.167 HPAR + 6 PAR
Propenylcyclohexane	672	OLE + 7 PAR
Ethyl-3-Ethoxypropionate	448	ETHR + 3 PAR
n-Heptane	600	0.083 HPAR + 6 PAR
1,3,5-Trimethylbenzene	44	XYL + 2 PAR
1,3,5-trimethylbenzene	44	XYL + 2 PAR
cis-1,3-dimethylcyclohexane	352	0.167 HPAR + 6 PAR
Acrylic Acid	1903	IVOC
2-methylhexane	194	0.083 HPAR + 6 PAR
n-Pentadecane	1049	IVOC
3-methylheptane	244	0.167 HPAR + 6 PAR
C9 Cycloalkanes	2170	0.33 HPAR + 5 PAR
n-Octane	604	0.33 HPAR + 5 PAR
Oxygenates	2215	ETHR + PAR
Triethanolamine	750	NONR
C11 Tetrasubstituted Benzenes	3208	IVOC
N-Octane	604	0.33 HPAR + 5 PAR
2-Pyrrolidone	3148	NONR
1-Ethyl-2-Propyl Cyclohexane	447	0.5 HPAR + 4 PAR
Methyldecene	553	OLE + 9 PAR
N-Propylbenzene	608	TOL + 2 PAR
C16 Branched Alkanes	1941	IVOC
Vinyl Acetate	768	OLE + 2 PAR
n-Nonane	603	0.33 HPAR + 5 PAR
Tetramethylpentanone	710	KET + 8 PAR
Ethylcyclohexane	450	0.33 HPAR + 5 PAR
Tetramethylbenzenes	23	IVOC
Methyl Ethyl Ketoxime	537	NONR
Isomers Of Dodecane	503	HPAR
T-Butylbenzene	703	TOL + 3 PAR
Propyl Acetate	674	ESTR + PAR
Trimethylhexene	759	OLE + 7 PAR

Compound Name	SPECIATE ID	CB6 & VCP Mapping
Diethylene Glycol Monomethyl Ether	534	ROH + PAR
Branched C10 Alkanes	3196	0.5 HPAR + 4 PAR
Peroxyacetic Acid	660	AACD
Dimethylheptanes	428	0.33 HPAR + 5 PAR
Ethylene Glycol Monopropyl Ether	458	ROH + PAR
Dimethylethylcyclohexane	427	0.5 HPAR + 4 PAR
C5 Branched Alkanes	3200	5 PAR
Propanoic Acid, 2-Methyl-2,2-Dimethyl-1-(1-Methylethyl)-1,3-Propanediyl Ester	3317	IVOC
C10 Dialkyl Benzenes	3256	XYL + 2 PAR
trans-1,3-dimethylcyclohexane	726	0.33 HPAR + 5 PAR
C14 Cycloalkanes	3230	0.67 IVOC + 0.33 HPAR
1,2,3-Trimethylbenzene	25	XYL + PAR
Dibasic Ester	3289	ESTR + 2 PAR
4-methylnonane	266	0.5 HPAR + 4 PAR
Propyl Heptene	675	OLE + 8 PAR
p-Ethyltoluene	94	XYL + PAR
1,2,3,5-Tetramethylbenzene	23	IVOC
o-Ethyltoluene	80	XYL + PAR
2-ethoxyethyl acetate (or cellosolve acetate)	173	ETHR + 2 PAR
C16 Cycloalkanes	3232	IVOC
p-Xylene	648	XYL
C12 Trisubstituted Benzenes	3211	XYL + PAR
Ketones - general	2137	KET + 4 PAR
2,6-dimethylheptane	160	0.33 HPAR + 5 PAR
Polytetrafluoroethylene	3314	NONR
Diacetone Alcohol	396	ROH + 2 PAR
Methylindans	2186	IVOC
Aliphatics	290	IVOC
Pentanedioic Acid, Dimethyl Ester	656	IVOC
Soybean Oil	3264	IVOC
1-Methyl-2-Ethylbenzene	80	XYL + PAR
Methyl Methacrylate	541	OLE + 2 PAR
Hydroxypropyl Methacrylate	3306	OLE + 3 PAR
C15 Branched Alkanes	1938	IVOC
Methylundecane	2199	HPAR
1,2,3-trimethylbenzene	25	XYL + PAR
3-methyldecane	243	0.75 HPAR + 2 PAR
n-Tetradecane	1051	0.67 IVOC + 0.33 HPAR
1,2,4-trimethylcyclopentane	31	0.167 HPAR + 6 PAR

Compound Name	SPECIATE ID	CB6 & VCP Mapping
Naphthalene	611	IVOC
Camphor	330	IVOC

Table S-3. Emissions of CB6 species for the for the Los Angeles box model scenario on July 31, 2011, in moles/day/km^2.

CB6 Species	Emissions (moles/day/km^2)
ACET	15.59
ALD2	5.25
ALDX	4.62
BENZ	8.34
CO	6952.66
ETH	41.44
ETHA	37.45
ETHY	13.66
ETOH	34.84
FORM	11.55
HONO	3.19
IOLE	13.87
ISOP	0.10
KET	4.68
MEOH	20.39
NO	410.69
NO2	49.12
OLE	29.18
PAR	1184.29
PRPA	17.26
TERP	1.61
TOL	41.46
NONR	75.47
XYL	28.39

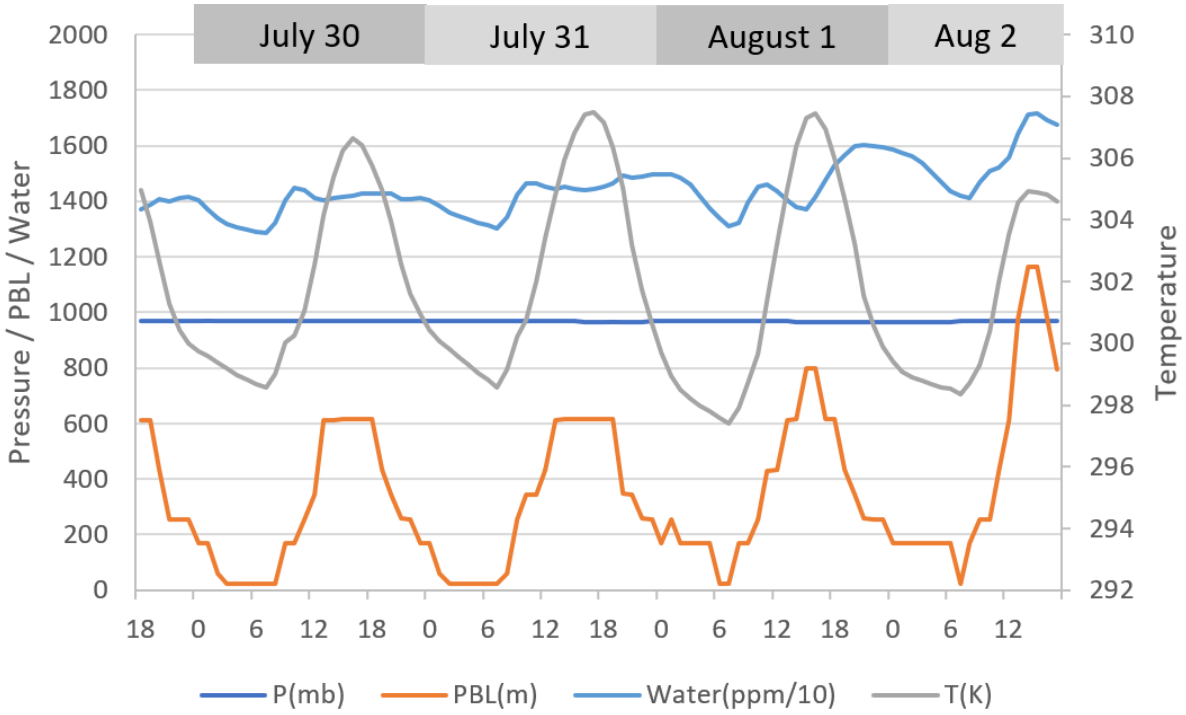

Figure S-1. Meteorological conditions for the Los Angeles box model scenario shown in local standard time for July 29 to August 2, 2011.

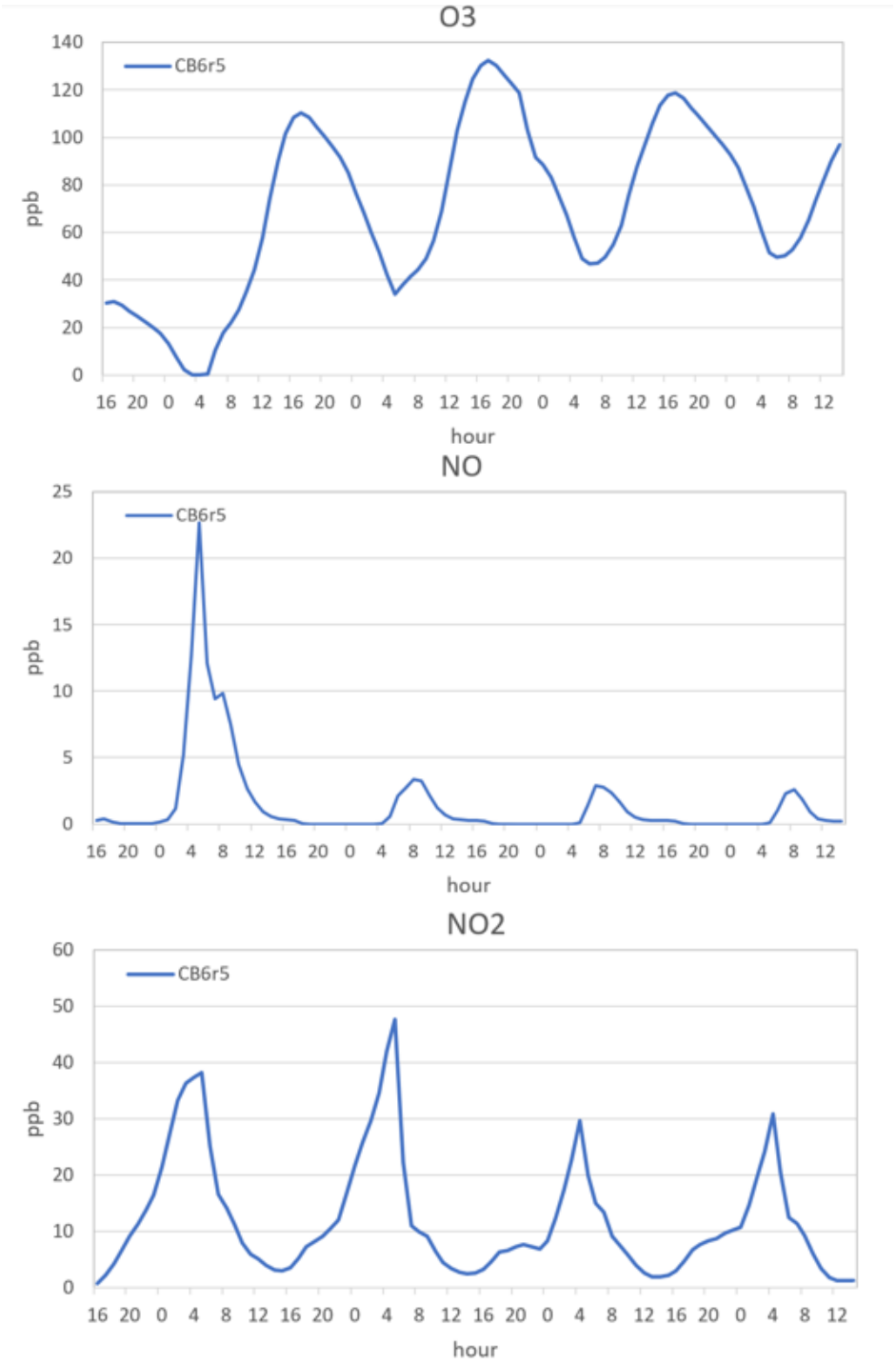

Figure S-2. Time series for O_3, NO and NO_2 in the Los Angeles box model scenario shown in local standard time for July 29 to August 2, 2011.