



## Supplement of

## Differences in the key volatile organic compound species between their emitted and ambient concentrations in ozone formation

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Fig. S1. Three monitoring sites in the Sichuan Basin (b), China (a). The red rectangles in panels (a) and (b) indicate the miniature map of panels (b) and (c), respectively. Wind vectors at local 8:00 am 4 September 2019 are from the European Centre for Medium-Range Weather Forecasts (https://www.ecmwf.int/) (c). The grey polygons indicate cities (c).



Fig. S2. Diurnal variations of surface net solar radiation at rural Deyang, suburban Chengdu, and forest Meishan from August to September 2019, respectively. Scatters and shaded envelopes are the mean and standard error (SE), respectively. The units are joules per square meter (J m<sup>-2</sup>). Data are from the European Centre for Medium-Range Weather Forecasts <u>https://www.ecmwf.int/</u>).

			I	kNO <sub>3</sub> or kO <sub>3</sub> (cm	<sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup> )		
	10	<sup>-18</sup> 10 <sup>°</sup>	<sup>-17</sup> <b>1</b> 0 <sup>-</sup>	<sup>-16</sup> 10 <sup>-</sup>	<sup>-15</sup> 10	-14 10	-13 10 <sup>-12</sup>
	_						
lsoprene (Carter, 2010)							
Styrene (Carter, 2010)							
1,3-Butadiene (Carter, 2010)						1	
trans-2-Butene (Carter, 2010)							
cis-2-Butene (Carter, 2010)							
Propylene (Carter, 2010)			]				
Ethylene (Atkinson and Arey, 2003)							
cis-2-Pentene (Carter, 2010)							
1-Butene (Carter, 2010)							
1-Hexene (Carter, 2010)							
1-Pentene (Carter, 2010)			]				kNO <sub>3</sub> kO <sub>3</sub>

Fig. S3. The reported reaction rate constants of 10 alkenes and styrene with  $NO_3$  radicals and  $O_3$  at 300K (Carter, 2010; Atkinson and Arey, 2003).



Fig. S4. The correlations between ambient concentrations of benzene and styrene during nighttime from August to September 2019. The slopes of solid and dotted lines indicate the emission ratios of benzene to isoprene and their uncertainties, respectively.



Fig. S5. The correlations between ambient concentrations of benzene and cis-2-butene or trans-2-butene during nighttime from August to September 2019, respectively. The slopes of solid and dotted lines indicate the emission ratios and their uncertainties, respectively.



25 Fig. S6. Diurnal variations of ratios of ambient concentrations of ethylbenzene to m,p-xylene, and estimated emission ratios. The black, red, and blue dots (a-c) and lines (d-f) indicate mean values, and shaded envelopes mark SD (a-f).



Fig. S7. The reported reaction rate constants of 99 VOCs with OH radicals at 300K. The kOH values for acetonitrile, m-diethylbenzene, pdiethylbenzene are cited (Atkinson and Arey, 2003; Atkinson, 2000), and the other VOCs (Carter, 2010). The kOH value of m,p-xylene is the average kOH value of m-xylene and p-xylene.



30 Fig. S8. The correlations between ambient concentrations of methyl vinyl ketone and isoprene during nighttime from August to September 2019. The slopes of solid and dotted lines indicate the emission ratios of benzene to isoprene and their uncertainties, respectively.



Fig. S9. The reported ratios (R) of J<sub>OVOC</sub> to [OH]kOH<sub>OVOC</sub> (de Gouw et al., 2018). The R values are established in the Los Angeles Basin for acetone, methyl ethyl ketone, n-hexanal, n-butanal, propanal, Acetaldehyde, and acrolein (de Gouw et al., 2018). According to similar chemical structures, the R values for methyl vinyl ketone and methacrolein refer to that of methyl ethyl ketone; the R values for 2-pentanone and 3-pentanone refer to the average of acetone and methyl ethyl ketone; and the R value for n-pentanal refers to the average of n-butanal and n-hexanal.



Fig. S10. Hourly OFP values based on ambient (a, c, and e) and emitted (b, d, and f) VOCs concentrations at Deyang, Chengdu, and Meishan from August to September 2019, respectively.



40 Fig. S11. Diurnal variations of OFP values based on emitted (a, c, and e) and ambient (b, d, and f) VOCs concentrations at Deyang, Chengdu, and Meishan from August to September 2019, respectively.

	Dey	vang	Cher	ngdu	Mei	shan
Species	[VOCs]	[e-VOCs]	[VOCs]	[e-VOCs]	[VOCs]	[e-VOCs]
Ethane (Alkane)	$4.25\pm1.80$	$4.26\pm1.79$	$3.03 \pm 1.21$	$3.04 \pm 1.21$	$3.36 \pm 1.03$	$3.37 \pm 1.03$
Propane	$2.70\pm2.33$	$2.73\pm2.33$	$2.55\pm2.08$	$2.58\pm2.08$	$1.46\pm0.70$	$1.47\pm0.70$
Isobutane	$0.79\pm0.59$	$0.81\pm0.59$	$0.65\pm0.47$	$0.66\pm0.47$	$0.38\pm0.14$	$0.38\pm0.14$
n-Butane	$1.24\pm0.95$	$1.27\pm0.95$	$1.14\pm0.93$	$1.18\pm0.93$	$0.62\pm0.30$	$0.63\pm0.31$
Isopentane	$0.91\pm0.71$	$0.94\pm0.72$	$0.89\pm0.53$	$0.94\pm0.54$	$0.64\pm0.43$	$0.65\pm0.45$
n-Pentane	$0.45\pm0.37$	$0.46\pm0.37$	$0.32\pm0.19$	$0.34\pm0.19$	$0.37\pm0.65$	$0.38\pm0.69$
2,2-Dimethylbutane	$0.12\pm0.48$	$0.12\pm0.48$	$0.03\pm0.02$	$0.03\pm0.02$	$0.02\pm0.01$	$0.02\pm0.01$
2,3-Dimethylbutane	$0.07\pm0.19$	$0.08\pm0.19$	$0.07\pm0.09$	$0.08\pm0.09$	$0.02\pm0.01$	$0.02\pm0.01$
2-Methylpentane	$0.20\pm0.14$	$0.21\pm0.14$	$0.23\pm0.18$	$0.24\pm0.18$	$0.11\pm0.07$	$0.11\pm0.07$
Cyclopentane	$0.04\pm0.04$	$0.04\pm0.04$	$0.07\pm0.03$	$0.08\pm0.04$	$0.07\pm0.03$	$0.07\pm0.03$
3-Methylpentane	$0.18\pm0.15$	$0.19\pm0.16$	$0.17\pm0.13$	$0.18\pm0.13$	$0.09\pm0.06$	$0.10\pm0.06$
n-Hexane	$0.26\pm0.26$	$0.28\pm0.28$	$0.26\pm0.28$	$0.28\pm0.28$	$0.11\pm0.09$	$0.11\pm0.09$
2,4-Dimethylpentane	$0.04\pm0.08$	$0.04\pm0.08$	$0.06\pm0.07$	$0.06\pm0.09$	$0.01\pm0.01$	$0.01\pm0.01$
Methylcyclopentane	$0.12\pm0.13$	$0.12\pm0.13$	$0.08\pm0.05$	$0.09\pm0.06$	$0.05\pm0.02$	$0.05\pm0.02$
2-Methylhexane	$0.06\pm0.04$	$0.07\pm0.05$	$0.06\pm0.06$	$0.07\pm0.06$	$0.03\pm0.02$	$0.03\pm0.02$
2,3-Dimethylpentane	$0.02\pm0.01$	$0.02\pm0.01$	$0.03\pm0.02$	$0.03\pm0.02$	$0.01\pm0.01$	$0.02\pm0.01$
3-Methylhexane	$0.06\pm0.04$	$0.07\pm0.05$	$0.08\pm0.07$	$0.09\pm0.08$	$0.03\pm0.03$	$0.04\pm0.03$
2,2,4-Trimethylpentane	$0.04\pm0.03$	$0.04\pm0.03$	$0.04\pm0.05$	$0.04\pm0.05$	$0.02\pm0.01$	$0.02\pm0.01$
n-Heptane	$0.08\pm0.05$	$0.08\pm0.06$	$0.10\pm0.10$	$0.11\pm0.10$	$0.04\pm0.04$	$0.05\pm0.04$
Methylcyclohexane	$0.17\pm0.20$	$0.19\pm0.20$	$0.10\pm0.10$	$0.11\pm0.11$	$0.03\pm0.03$	$0.03\pm0.03$
2,3,4-Trimethylpentane	$0.07\pm0.24$	$0.07\pm0.24$	$0.02\pm0.02$	$0.02\pm0.02$	$0.01\pm0.00$	$0.01\pm0.00$
2-Methylheptane	$0.02\pm0.02$	$0.03\pm0.02$	$0.02\pm0.01$	$0.02\pm0.01$	$0.01\pm0.00$	$0.01\pm0.00$
3-Methylheptane	$0.02\pm0.01$	$0.02\pm0.02$	$0.02\pm0.01$	$0.02\pm0.01$	$0.01\pm0.00$	$0.01\pm0.00$
Cyclohexane	$0.05\pm0.04$	$0.06\pm0.04$	$0.05\pm0.11$	$0.06\pm0.11$	$0.02\pm0.02$	$0.02\pm0.02$
n-Octane	$0.06\pm0.05$	$0.07\pm0.05$	$0.04\pm0.03$	$0.05\pm0.03$	$0.02\pm0.01$	$0.02\pm0.02$
n-Nonane	$0.03\pm0.03$	$0.04\pm0.03$	$0.03\pm0.02$	$0.04\pm0.02$	$0.02\pm0.01$	$0.02\pm0.01$
n-Decane	$0.03\pm0.02$	$0.04\pm0.03$	$0.02\pm0.01$	$0.02\pm0.01$	$0.02\pm0.03$	$0.02\pm0.03$
n-Undecane	$0.05\pm0.03$	$0.06\pm0.05$	$0.02\pm0.01$	$0.02\pm0.02$	$0.01\pm0.01$	$0.01\pm0.01$
n-Dodecane	$0.26\pm0.36$	$0.37\pm0.70$	$0.02\pm0.03$	$0.03\pm0.05$	$0.05\pm0.04$	$0.06\pm0.05$

Table S1 The amibient and emitted concentrations of VOCs species (Mean  $\pm$  SD; ppbv) during summer.

	Dey	rang	Che	ngdu	Mei	shan
Species	[VOCs]	[e-VOCs]	[VOCs]	[e-VOCs]	[VOCs]	[e-VOCs]
Ethylene (Alkene)	$2.15\pm1.64$	$2.32 \pm 1.65$	$1.60\pm1.05$	$1.76 \pm 1.04$	$1.83 \pm 1.19$	$1.91 \pm 1.19$
Propylene	$0.47\pm0.50$	$0.62\pm0.53$	$0.28\pm0.23$	$0.40\pm0.28$	$0.32\pm0.34$	$0.36\pm0.35$
trans-2-Butene	$0.03\pm0.04$	$0.52\pm0.92$	$0.02\pm0.05$	$0.14\pm0.30$	$0.01\pm0.01$	$0.06\pm0.09$
1-Butene	$0.13\pm0.14$	$0.22\pm0.31$	$0.56\pm0.69$	$1.34\pm2.06$	$0.13\pm0.11$	$0.19\pm0.21$
cis-2-Butene	$0.17\pm0.10$	$1.21\pm2.02$	$0.02\pm0.03$	$0.08\pm0.19$	$0.03\pm0.02$	$0.07\pm0.05$
1,3-Butadiene	$0.04\pm0.03$	$0.13\pm0.19$	$0.03\pm0.03$	$0.17\pm0.47$	$0.05\pm0.06$	$0.10\pm0.13$
1-Pentene	$0.03\pm0.03$	$0.04\pm0.03$	$0.02\pm0.02$	$0.04\pm0.05$	$0.02\pm0.03$	$0.03\pm0.03$
trans-2-Pentene	$0.02\pm0.04$	$0.19\pm0.36$	$0.01\pm0.02$	$0.05\pm0.14$	$0.00\pm0.00$	$0.01\pm0.02$
Isoprene	$0.26\pm0.26$	$0.96\pm0.81$	$0.47\pm0.62$	$1.28 \pm 1.25$	$1.48\pm2.54$	$3.28 \pm 4.26$
cis-2-Pentene	$0.01\pm0.02$	$0.19\pm0.53$	$0.01\pm0.01$	$0.09\pm0.31$	$0.01\pm0.01$	$0.04\pm0.12$
1-Hexene	$0.03\pm0.03$	$0.05\pm0.05$	$0.01\pm0.01$	$0.03\pm0.05$	$0.02\pm0.03$	$0.03\pm0.04$
Acetylene	$2.54\pm2.00$	$2.57\pm2.02$	$2.11 \pm 1.23$	$2.13 \pm 1.24$	$1.70\pm0.70$	$1.70\pm0.70$
Acetonitrile	$0.33\pm0.17$	$0.33\pm0.17$	$0.41\pm0.67$	$0.41\pm0.67$	$0.31\pm0.12$	$0.31\pm0.12$
CFC-11 (Halocarbon)	$1.44 \pm 1.24$	$1.44 \pm 1.24$	$0.23\pm0.32$	$0.23\pm0.32$	$0.22\pm0.03$	$0.22\pm0.03$
CFC-113	$0.06\pm0.01$	$0.06\pm0.01$	$0.08\pm0.01$	$0.08\pm0.01$	$0.08\pm0.00$	$0.08\pm0.00$
CFC-114	$0.02\pm0.01$	$0.02\pm0.01$	$0.01\pm0.00$	$0.01\pm0.00$	$0.02\pm0.00$	$0.02\pm0.00$
Chloromethane	$0.40\pm0.16$	$0.40\pm0.16$	$0.62\pm0.24$	$0.63\pm0.24$	$0.83\pm0.72$	$0.83\pm0.72$
Vinyl chloride	$0.04\pm0.10$	$0.04\pm0.12$	$0.04\pm0.14$	$0.04\pm0.14$	$0.02\pm0.06$	$0.03\pm0.06$
Bromomethane	$0.01\pm0.00$	$0.01\pm0.00$	$0.01\pm0.00$	$0.01\pm0.00$	$0.01\pm0.00$	$0.01\pm0.00$
Chloroethane	$0.02\pm0.02$	$0.02\pm0.02$	$0.02\pm0.02$	$0.02\pm0.02$	$0.02\pm0.01$	$0.02\pm0.01$
1,1-Dichloroethene	$0.00\pm0.01$	$0.00\pm0.01$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Dichloromethane	$1.50\pm1.66$	$1.50\pm1.66$	$2.80\pm3.09$	$2.80\pm3.09$	$0.84 \pm 0.74$	$0.84\pm0.74$
1,1-Dichloroethane	$0.16\pm0.66$	$0.16\pm0.66$	$0.03\pm0.03$	$0.03\pm0.03$	$0.03\pm0.02$	$0.03\pm0.02$
Chloroform	$0.09\pm0.05$	$0.09\pm0.05$	$0.10\pm0.12$	$0.10\pm0.12$	$0.08\pm0.03$	$0.08\pm0.03$
1,1,1-Trichloroethane	$0.00\pm0.01$	$0.00\pm0.01$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Carbon tetrachloride	$0.12\pm0.06$	$0.12\pm0.06$	$0.08\pm0.01$	$0.08\pm0.01$	$0.11\pm0.00$	$0.11\pm0.00$
1,2-Dichloroethane	$0.59\pm0.59$	$0.59\pm0.59$	$0.53\pm0.45$	$0.53\pm0.45$	$0.60\pm0.45$	$0.60\pm0.45$
Trichloroethylene	$0.04\pm0.11$	$0.04\pm0.11$	$0.04\pm0.04$	$0.04\pm0.04$	$0.01\pm0.04$	$0.02\pm0.04$
1,2-Dichloropropane	$0.18\pm0.26$	$0.18\pm0.26$	$0.25\pm0.24$	$0.25\pm0.24$	$0.12\pm0.10$	$0.12\pm0.10$

Continued Table S1 The amibient and emitted concentrations of VOCs species (Mean ± SD; ppbv) during summ	mer.
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Surviv	Dey	ang	Cher	ngdu	Mei	shan
Species	[VOCs]	[e-VOCs]	[VOCs]	[e-VOCs]	[VOCs]	[e-VOCs]
Bromodichloromethane	$0.01\pm0.02$	$0.01\pm0.02$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
trans-1,3-Dichloropropene	$0.01\pm0.02$	$0.01\pm0.02$	$0.00\pm0.00$	$0.01\pm0.00$	$0.00\pm0.01$	$0.00\pm0.01$
cis-1,3-Dichloropropene	$0.04\pm0.18$	$0.05\pm0.19$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
1,1,2-Trichloroethane	$0.02\pm0.01$	$0.02\pm0.01$	$0.02\pm0.02$	$0.02\pm0.02$	$0.01\pm0.01$	$0.01\pm0.01$
Tetrachloroethylene	$0.02\pm0.02$	$0.02\pm0.02$	$0.05\pm0.04$	$0.05\pm0.04$	$0.01\pm0.01$	$0.01\pm0.01$
1,2-Dibromoethane	$0.00\pm0.01$	$0.00\pm0.01$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Chlorobenzene	$0.01\pm0.01$	$0.01\pm0.01$	$0.01\pm0.00$	$0.01\pm0.00$	$0.01\pm0.00$	$0.01\pm0.00$
1,3-Dichlorobenzene	$0.09\pm0.04$	$0.09\pm0.04$	$0.02\pm0.01$	$0.02\pm0.01$	$0.02\pm0.00$	$0.02\pm0.00$
1,4-Dichlorobenzene	$0.03\pm0.03$	$0.03\pm0.03$	$0.01\pm0.01$	$0.01\pm0.01$	$0.01\pm0.00$	$0.01\pm0.00$
1,2-Dichlorobenzene	$0.01\pm0.02$	$0.01\pm0.02$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Benzyl chloride	$0.01\pm0.02$	$0.01\pm0.02$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
cis-1,2-Dichloroethene	$0.02\pm0.07$	$0.02\pm0.07$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Benzene (Aromatic)	$0.42\pm0.22$	$0.43\pm0.22$	$0.44\pm0.20$	$0.45\pm0.21$	$0.47\pm0.17$	$0.47\pm0.17$
Toluene	$0.73\pm0.59$	$0.78\pm0.60$	$0.93\pm0.74$	$1.00\pm0.78$	$0.36\pm0.25$	$0.37\pm0.26$
Ethylbenzene	$0.26\pm0.28$	$0.28\pm0.28$	$0.46\pm0.43$	$0.50\pm0.45$	$0.18\pm0.12$	$0.19\pm0.12$
o-Xylene	$0.28\pm0.36$	$0.31\pm0.37$	$0.52\pm0.52$	$0.60\pm0.57$	$0.20\pm0.15$	$0.22\pm0.15$
m,p-Xylene	$0.64\pm0.83$	$0.77\pm0.84$	$1.30\pm1.30$	$1.58 \pm 1.44$	$0.48\pm0.36$	$0.53\pm0.37$
Styrene	$0.18\pm0.16$	$0.87 \pm 1.75$	$0.15\pm0.19$	$0.50\pm0.70$	$0.09\pm0.05$	$0.20\pm0.15$
Isopropylbenzene	$0.02\pm0.02$	$0.02\pm0.02$	$0.01\pm0.01$	$0.01\pm0.01$	$0.01\pm0.00$	$0.01\pm0.00$
n-Propylbenzene	$0.02\pm0.02$	$0.02\pm0.02$	$0.02\pm0.01$	$0.02\pm0.01$	$0.01\pm0.01$	$0.01\pm0.01$
o-Ethyltoluene	$0.17\pm0.68$	$0.18\pm0.68$	$0.02\pm0.01$	$0.03\pm0.01$	$0.02\pm0.01$	$0.02\pm0.01$
m-Ethyltoluene	$0.04\pm0.05$	$0.05\pm0.05$	$0.04\pm0.03$	$0.05\pm0.03$	$0.02\pm0.01$	$0.02\pm0.02$
p-Ethyltoluene	$0.10\pm0.46$	$0.10\pm0.46$	$0.02\pm0.02$	$0.03\pm0.02$	$0.01\pm0.01$	$0.01\pm0.01$
1,3,5-Trimethylbenzene	$0.02\pm0.04$	$0.07\pm0.14$	$0.02\pm0.01$	$0.10\pm0.26$	$0.02\pm0.01$	$0.03\pm0.03$
1,2,4-Trimethylbenzene	$0.07\pm0.07$	$0.10\pm0.09$	$0.06\pm0.05$	$0.10\pm0.08$	$0.03\pm0.02$	$0.04\pm0.02$
1,2,3-Trimethylbenzene	$0.02\pm0.02$	$0.03\pm0.03$	$0.02\pm0.01$	$0.04\pm0.04$	$0.02\pm0.01$	$0.02\pm0.01$
m-Diethylbenzene	$0.02\pm0.07$	$0.03\pm0.07$	$0.01\pm0.01$	$0.01\pm0.01$	$0.00\pm0.00$	$0.00\pm0.00$
p-Diethylbenzene	$0.02\pm0.01$	$0.02\pm0.01$	$0.02\pm0.02$	$0.02\pm0.02$	$0.01\pm0.01$	$0.01\pm0.01$
Acetaldehyde (OVOC)	$2.49 \pm 1.55$	$2.08 \pm 1.10$	$3.89 \pm 4.38$	$3.31\pm2.49$	$1.83\pm2.08$	$1.55 \pm 1.44$

Service	Deya	ang	Cher	Chengdu Meishan		shan
Species	[VOCs]	[e-VOCs]	[VOCs]	[e-VOCs]	[VOCs]	[e-VOCs]
Acrolein	$0.13\pm0.08$	$0.12\pm0.08$	$0.07\pm0.05$	$0.07\pm0.05$	$0.09\pm0.12$	$0.09\pm0.12$
Propanal	$0.27\pm0.18$	$0.22\pm0.13$	$0.13\pm0.08$	$0.12\pm0.06$	$0.17\pm0.12$	$0.15\pm0.10$
n-Butanal	$0.17\pm0.26$	$0.14\pm0.25$	$0.04\pm0.03$	$0.03\pm0.02$	$0.07\pm0.04$	$0.07\pm0.03$
n-Pentanal	$0.15\pm0.23$	$0.14\pm0.23$	$0.06\pm0.04$	$0.04\pm0.03$	$0.04\pm0.03$	$0.04\pm0.03$
n-Hexanal	$0.78\pm0.87$	$0.83\pm0.66$	$0.19\pm0.20$	$0.14\pm0.11$	$0.18\pm0.09$	$0.16\pm0.08$
Acetone	$5.38\pm3.95$	$4.84 \pm 1.87$	$3.14 \pm 1.25$	$2.78 \pm 1.13$	$3.05 \pm 1.71$	$2.55 \pm 1.39$
Methyl vinyl ketone	$0.29\pm0.21$	$0.17\pm0.17$	$0.18\pm0.20$	$0.10\pm0.14$	$0.37\pm0.50$	$0.17\pm0.26$
Methyl ethyl ketone	$0.68\pm0.41$	$0.62\pm0.32$	$0.50\pm0.28$	$0.45\pm0.23$	$0.44\pm0.23$	$0.38 \pm 0.19$
2-Pentanone	$0.12\pm0.13$	$0.11\pm0.09$	$0.03\pm0.01$	$0.02\pm0.01$	$0.03\pm0.02$	$0.03\pm0.01$
3-Pentanone	$0.04\pm0.04$	$0.04\pm0.03$	$0.02\pm0.01$	$0.01\pm0.01$	$0.01\pm0.01$	$0.01\pm0.01$
Methyl tert-butyl ether	$0.27\pm0.27$	$0.27\pm0.27$	$0.09\pm0.08$	$0.09 \pm 0.08$	$0.14\pm0.07$	$0.15\pm0.08$

Continued Table S1 The amibient and emitted concentrations of VOCs species (Mean ± SD; ppbv) during summer.

		$\Delta$ [VOCs]	
Species	Deyang	Chengdu	Meishan
cis-2-Butene (Alkene)	$1.04\pm2.02$	$0.06\pm0.18$	$0.04\pm0.04$
Isoprene	$0.70\pm0.65$	$0.81\pm0.84$	$1.79\pm2.20$
trans-2-Butene	$0.49\pm0.90$	$0.12\pm0.30$	$0.05\pm0.08$
cis-2-Pentene	$0.18\pm0.53$	$0.08\pm0.31$	$0.03\pm0.12$
Ethylene	$0.17\pm0.19$	$0.16\pm0.20$	$0.08\pm0.10$
trans-2-Pentene	$0.17\pm0.33$	$0.04\pm0.14$	$0.01\pm0.01$
Propylene	$0.15\pm0.17$	$0.13\pm0.18$	$0.05\pm0.05$
1-Butene	$0.09\pm0.22$	$0.78 \pm 1.72$	$0.05\pm0.14$
1,3-Butadiene	$0.09\pm0.18$	$0.14\pm0.47$	$0.05\pm0.08$
1-Hexene	$0.02\pm0.04$	$0.02\pm0.05$	$0.01\pm0.01$
1-Pentene	$0.01\pm0.02$	$0.02\pm0.04$	$0.01\pm0.01$
Styrene (Aromatic)	$0.70\pm1.76$	$0.38\pm0.69$	$0.11\pm0.15$
m,p-Xylene	$0.12\pm0.22$	$0.28\pm0.50$	$0.06\pm0.12$
Toluene	$0.05\pm0.09$	$0.07\pm0.12$	$0.01\pm0.03$
1,3,5-Trimethylbenzene	$0.04\pm0.14$	$0.08\pm0.26$	$0.01\pm0.03$
o-Xylene	$0.04\pm0.07$	$0.08\pm0.15$	$0.02\pm0.04$
1,2,4-Trimethylbenzene	$0.03\pm0.07$	$0.04\pm0.08$	$0.01\pm0.02$
Ethylbenzene	$0.02\pm0.04$	$0.04\pm0.07$	$0.01\pm0.02$
1,2,3-Trimethylbenzene	$0.01\pm0.03$	$0.02\pm0.04$	$0.00\pm0.01$
m-Ethyltoluene	$0.01\pm0.01$	$0.01\pm0.02$	$0.00\pm0.01$
Benzene	$0.01\pm0.01$	$0.01\pm0.01$	$0.00\pm0.01$
p-Ethyltoluene	$0.00\pm0.00$	$0.00\pm0.01$	$0.00\pm0.00$
o-Ethyltoluene	$0.00\pm0.00$	$0.00\pm0.01$	$0.00\pm0.00$
m-Diethylbenzene	$0.00\pm0.01$	$0.00\pm0.00$	$0.00\pm0.00$
p-Diethylbenzene	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
n-Propylbenzene	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Isopropylbenzene	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
n-Dodecane (Alkane)	$0.11\pm0.40$	$0.01\pm0.03$	$0.00\pm0.01$
Isopentane	$0.03\pm0.06$	$0.05\pm0.07$	$0.01\pm0.04$

		$\Delta$ [VOCs]	
Species	Deyang	Chengdu	Meishan
Propane	$0.03\pm0.05$	$0.03\pm0.05$	$0.01\pm0.02$
n-Butane	$0.03\pm0.05$	$0.03\pm0.05$	$0.01\pm0.02$
n-Hexane	$0.02\pm0.03$	$0.01\pm0.03$	$0.00\pm0.01$
n-Pentane	$0.02\pm0.03$	$0.02\pm0.03$	$0.01\pm0.06$
Isobutane	$0.02\pm0.03$	$0.02\pm0.02$	$0.01\pm0.01$
Methylcyclohexane	$0.01\pm0.03$	$0.01\pm0.02$	$0.00\pm0.00$
n-Undecane	$0.01\pm0.03$	$0.00\pm0.01$	$0.00\pm0.00$
Ethane	$0.01\pm0.02$	$0.01\pm0.02$	$0.00\pm0.01$
2-Methylpentane	$0.01\pm0.02$	$0.01\pm0.02$	$0.00\pm0.01$
3-Methylpentane	$0.01\pm0.02$	$0.01\pm0.02$	$0.00\pm0.01$
n-Octane	$0.01\pm0.01$	$0.01\pm0.01$	$0.00\pm0.00$
n-Heptane	$0.01\pm0.01$	$0.01\pm0.02$	$0.00\pm0.00$
Methylcyclopentane	$0.01\pm0.01$	$0.01\pm0.01$	$0.00\pm0.00$
2-Methylhexane	$0.01\pm0.01$	$0.01\pm0.01$	$0.00\pm0.00$
3-Methylhexane	$0.01\pm0.01$	$0.01\pm0.01$	$0.00\pm0.00$
n-Decane	$0.00\pm0.01$	$0.00\pm0.01$	$0.00\pm0.00$
n-Nonane	$0.00\pm0.01$	$0.00\pm0.01$	$0.00\pm0.00$
Cyclohexane	$0.00\pm0.01$	$0.00\pm0.01$	$0.00\pm0.00$
2,3-Dimethylbutane	$0.00\pm0.00$	$0.00\pm0.01$	$0.00\pm0.00$
2-Methylheptane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
3-Methylheptane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
2,3-Dimethylpentane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
2,2,4-Trimethylpentane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
2,3,4-Trimethylpentane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
2,4-Dimethylpentane	$0.00\pm0.00$	$0.01\pm0.02$	$0.00\pm0.00$
2,2-Dimethylbutane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Cyclopentane	$0.00\pm0.00$	$0.01\pm0.01$	$0.00\pm0.00$
n-Hexanal (OVOC)	$0.04\pm0.57$	$\textbf{-0.04} \pm 0.17$	$\textbf{-0.01} \pm 0.05$

Continued Table 52 The differences between emitted and ambient vOCs concentrations (Mean $\pm$ SD; ppbv) during summe
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		$\Delta$ [VOCs]	
Species	Deyang	Chengdu	Meishan
Methyl tert-butyl ether	$0.01\pm0.02$	$0.00\pm0.01$	$0.00\pm0.01$
Methacrolein	$0.00\pm0.00$	$\textbf{-0.03} \pm 0.06$	$\textbf{-0.02}\pm0.13$
3-Pentanone	$-0.01 \pm 0.03$	$0.00\pm0.00$	$0.00\pm0.00$
Acrolein	$-0.01 \pm 0.03$	$\textbf{-0.00}\pm0.02$	$\textbf{-0.00}\pm0.02$
2-Pentanone	$-0.01 \pm 0.09$	$\textbf{-0.00} \pm 0.01$	$\textbf{-0.00} \pm 0.01$
n-Pentanal	$-0.01 \pm 0.06$	$\textbf{-0.01} \pm 0.03$	$\textbf{-0.00}\pm0.02$
n-Butanal	$\textbf{-0.03}\pm0.06$	$\textbf{-0.01} \pm 0.02$	$\textbf{-0.01} \pm 0.02$
Propanal	$-0.05 \pm 0.11$	$\textbf{-0.02}\pm0.05$	$-0.02\pm0.06$
Methyl ethyl ketone	$-0.06 \pm 0.22$	$-0.05 \pm 0.17$	$\textbf{-0.06} \pm 0.14$
Methyl vinyl ketone	$-0.12 \pm 0.19$	$\textbf{-0.05} \pm 0.14$	$\textbf{-0.18} \pm 0.44$
Acetaldehyde	$-0.42 \pm 0.91$	$-0.58\pm3.49$	$-0.28 \pm 1.44$
Acetone	$-0.54 \pm 3.63$	$\textbf{-0.36} \pm 0.92$	$-0.50 \pm 1.13$
Acetylene	$0.02\pm0.04$	$0.02\pm0.03$	$0.01\pm0.01$
Vinyl chloride (Halocarbon)	$0.00\pm0.02$	$0.00\pm0.01$	$0.00\pm0.00$
cis-1,3-Dichloropropene	$0.00\pm0.04$	$0.00\pm0.00$	$0.00\pm0.00$
Dichloromethane	$0.00\pm0.01$	$0.00\pm0.01$	$0.00\pm0.00$
1,2-Dichloroethane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
1,2-Dichloropropane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
trans-1,3-Dichloropropene	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Trichloroethylene	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
1,1-Dichloroethene	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Chloromethane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
1,1-Dichloroethane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Chloroethane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Chloroform	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Chlorobenzene	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Tetrachloroethylene	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
1,1,2-Trichloroethane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
1,2-Dibromoethane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$

Continued Table S2 The differences between emitted and ambient VOCs concentrations (Mean ± SD; ppbv) during sum	mer
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		$\Delta$ [VOCs]	
Species	Deyang	Chengdu	Meishan
Bromomethane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
1,1,1-Trichloroethane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
CFC-114	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
cis-1,2-Dichloroethene	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
CFC-11	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Bromodichloromethane	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
1,4-Dichlorobenzene	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Benzyl chloride	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
1,2-Dichlorobenzene	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
1,3-Dichlorobenzene	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Carbon tetrachloride	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
CFC-113	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$
Acetonitrile	$0.00\pm0.00$	$0.00\pm0.00$	$0.00\pm0.00$

Continued Table 52 The differences between emitted and ambient vOCs concentrations (wean $\pm$ 5D, ppbv) during summer	Continue	1 Table S2	The differences	between e	mitted and	ambient	VOCs	concentrations	(Mean $\pm$ SD;	ppbv) during	summer.
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Name	Sampling time	VOCs number	Type of sites	References
Acetaldehyde, Ethylene, and m,p-Xylene; m,p-Xylene, Toluene, and Ethylene; Ethylene, m,p-Xylene, and Acetaldehyde; Acetaldehyde, m,p-Xylene, and Ethylene; Ethylene, Acetaldehyde, and m,p-Xylene; Ethylene, Acetaldehyde, and Toluene	May 2016 – January 2017	99	Urban Chengdu	(Tan et al., 2020b)
Ethylene, trans-2-Pentene, and Toluene	August 28, 2016 – October 7, 2016	94	Urban Chengdu	(Deng et al., 2019)
Ethylene, Propylene, and m,p-Xylene	October 27, 2016 - September 30, 2017	55	Urban Chengdu	(Song et al., 2018)
Propylene, 2-Butene, and 1-Butene; m,p-Xylene, Acetaldehyde, and Toluene; Acetaldehyde, m,p-Xylene, and o-Xylene	July 31, 2017 – August 31, 2017	99	Urban Chengdu	(Tan et al., 2020a)
m,p-Xylene, Toluene, and Ethylene; Ethylene, m,p-Xylene, and Toluene	June 1, 2018 – June 29, 2018	90	Urban Chengdu	(Xiong et al., 2021)
Ethylene, m,p-Xylene, and Toluene; m,p-Xylene, Toluene, and Ethylene; m,p-Xylene, Ethylene, and o-Xylene; Ethylene, m,p-Xylene, and Propylene	January 1, 2019 – December 31, 2019	56	Urban Chengdu	(Kong et al., 2023)
m,p-Xylene, Toluene, and o-Xylene	June to August 2019	122	Urban Chengdu	(Wang et al., 2023)
Acetaldehyde and Isoprene	August 20, 2019 – September 12, 2019	10	Rural Deyang	(Chen et al., 2021)

Table S3 The reported top three VOCs species contributing to OFP based on ambient concentrations in the Sichuan Basin, China.

## **Supplementary References**

Atkinson, R.: Atmospheric chemistry of VOCs and NO<sub>x</sub>, Atmos. Environ., 34, 2063-2101, 10.1016/s1352-2310(99)00460-4, 2000.

60 Atkinson, R. and Arey, J.: Atmospheric degradation of volatile organic compounds, Chem. Rev., 103, 4605-4638, 10.1021/cr0206420, 2003.

Carter, W. P. L.: Development of the SAPRC-07 chemical mechanism, Atmos. Environ., 44, 5324-5335, 10.1016/j.atmosenv.2010.01.026, 2010.

Chen, M. L., Wang, S. N., Chen, T. S., Zhu, B., Peng, C., Zhou, J. W., Che, H. X., Huang, R. H., Yang, F. M., Liu, H. F., Tan,
Q. W., Han, L., Chen, J. H., Lu, K. D., Chen, Y.: Source analysis of atmospheric oxygenated volatile organic compounds in the typical regions of Southwest China during the summer, Environ. Sci., 42, 10.13227/j.hjkx.202010101, 2648-2658, 2021.

de Gouw, J. A., Gilman, J. B., Kim, S. W., Alvarez, S. L., Dusanter, S., Graus, M., Griffith, S. M., Isaacman-VanWertz, G., Kuster, W. C., Lefer, B. L., Lerner, B. M., McDonald, B. C., Rappenglück, B., Roberts, J. M., Stevens, P. S., Stutz, J., Thalman, R., Veres, P. R., Volkamer, R., Warneke, C., Washenfelder, R. A., and Young, C. J.: Chemistry of volatile organic compounds in the Los Angeles Basin: formation of oxygenated compounds and determination of emission ratios, J. Geophys. Res.: Atmos.,

123, 2298-2319, 10.1002/2017jd027976, 2018.

70

85

90

Deng, Y. Y., Li, J., Li, Y. Q., Wu, R. R., and Xie, S. D.: Characteristics of volatile organic compounds, NO<sub>2</sub>, and effects on ozone formation at a site with high ozone level in Chengdu, J. Environ. Sci., 75, 334-345, 10.1016/j.jes.2018.05.004, 2019.

Kong, L., Zhou, L., Chen, D. Y., Luo, L., Xiao, K., Chen, Y., Liu, H. F., Tan, Q. W., and Yang, F. M.: Atmospheric oxidation
 capacity and secondary pollutant formation potentials based on photochemical loss of VOCs in a megacity of the Sichuan
 Basin, China, Sci. Total Environ., 901, 166259, 10.1016/j.scitotenv.2023.166259, 2023.

Song, M. D., Tan, Q. W., Feng, M., Qu, Y., Liu, X. G., An, J. L., and Zhang, Y. H.: Source apportionment and secondary transformation of atmospheric nonmethane hydrocarbons in Chengdu, southwest China, J. Geophys. Res.: Atmos., 123, 9741-9763, 10.1029/2018jd028479, 2018.

80 Tan, Q. W., Zhou, L., Liu, H. F., Feng, M., Qiu, Y., Yang, F. M., Jiang, W. J., and Wei, F. S.: Observation-based summer O<sub>3</sub> control effect evaluation: a case study in Chengdu, a megacity in Sichuan Basin, China, Atmosphere, 11, 1278, 10.3390/atmos11121278, 2020a.

Tan, Q. W., Liu, H. F., Xie, S. D., Zhou, L., Song, T. L., Shi, G. M., Jiang, W. J., Yang, F. M., and Wei, F. S.: Temporal and spatial distribution characteristics and source origins of volatile organic compounds in a megacity of Sichuan Basin, China, Environ. Res., 185, 109478, 10.1016/j.envres.2020.109478, 2020b.

Wang, D. C., Zhou, J. B., Han, L., Tian, W. N., Wang, C. H., Li, Y. J., and Chen, J. H.: Source apportionment of VOCs and ozone formation potential and transport in Chengdu, China, Atmos. Pollut. Res., 14, 101730, 10.1016/j.apr.2023.101730, 2023.

Xiong, C., Wang, N., Zhou, L., Yang, F. M., Qiu, Y., Chen, J. H., Han, L., and Li, J. J.: Component characteristics and source apportionment of volatile organic compounds during summer and winter in downtown Chengdu, southwest China, Atmos. Environ., 258, 118485, 10.1016/j.atmosenv.2021.118485, 2021.

22