

Supplementary information

# Ozone profiles, precursors, and Vertical Distribution in Urban Lhasa, Tibetan Plateau

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NO	Compounds	CAS NO	Category	MDL	R <sup>2</sup>	Accuracy
1	ethane	74-84-0	alkane	0.016	0.9977	0.87%
2	ethylene	74-85-1	alkene	0.026	0.9961	1.01%
3	propane	74-98-6	alkane	0.02	0.9977	0.71%
4	propylene	115-07-1	alkene	0.031	0.9966	0.83%
5	isobutane	75-28-5	alkane	0.02	0.9971	0.77%
6	acetylene	74-86-2	alkyne	0.02	0.9971	0.65%
7	N-Butane	106-97-8	alkane	0.022	0.9975	0.74%
8	Trans-2-butene	624-64-6	alkene	0.011	0.9966	0.53%
9	1-Butene	106-98-9	alkene	0.011	0.9967	0.36%
10	cis-2-butene	590-18-1	alkene	0.009	0.9962	0.74%
11	cyclopentane	287-92-3	alkane	0.009	0.9965	0.49%
12	Isopentane	78-78-4	alkane	0.005	0.9973	0.77%
13	pentane	109-66-0	alkane	0.005	0.9971	0.50%
14	Freon 12	75-71-8	Halogenated hydrocarbons	0.05	0.9996	2.75%
15	Freon 114	76-14-2	Halogenated hydrocarbons	0.002	0.9996	2.87%
16	methyl chloride	74-87-3	Halogenated hydrocarbons	0.007	0.9969	3.76%
17	vinyl chloride	27398	Halogenated hydrocarbons	0.042	0.9996	1.71%
18	1,3-Butadiene	106-99-0	alkene	0.037	0.9995	2.98%
19	methyl bromide	74-83-9	Halogenated hydrocarbons	0.024	0.9994	2.98%
20	Chloroethane	75-00-3	Halogenated hydrocarbons	0.031	0.9995	3.27%
21	Freon 11	75-69-4	Halogenated hydrocarbons	0.046	0.9998	3.77%

22	1-Pentene	109-67-1	alkene	0.009	0.9977	3.27%
23	Trans-2-pentene	646-04-8	alkene	0.004	0.9983	3.80%
24	isoprene	78-79-5	Natural source	0.02	0.9971	3.13%
25	Cis-2-pentene	627-20-3	alkene	0.016	0.9975	3.75%
26	acrolein	107-02-8	OVOCs	0.05	0.9965	4.34%
27	1,1-Dichloroethylene	75-35-4	Halogenated hydrocarbons	0.031	0.9997	3.85%
28	Freon 113	76-13-1	Halogenated hydrocarbons	0.027	0.9998	2.08%
29	2,2-Dimethylbutane	75-83-2	alkane	0.005	0.9979	3.25%
30	acetone	67-64-1	OVOCs	0.05	0.9965	4.15%
31	carbon disulfide	75-15-0	Organic sulfur	0.033	0.9997	4.37%
32	isopropanol	67-63-0	OVOCs	0.009	0.9981	4.92%
33	2,3-Dimethylbutane	79-29-8	alkane	0.013	0.997	3.28%
34	dichloromethane	75-09-2	Halogenated hydrocarbons	0.037	0.9995	3.94%
35	2-Methylpentane	107-83-5	alkane	0.04	0.995	4.86%
36	3-Methylpentane	96-14-0	alkane	0.007	0.9974	3.45%
37	Methyl tert-butyl ether	1634-04-4	OVOCs	0.015	0.9992	3.59%
38	1-Hexene	592-41-6	alkene	0.011	0.9977	4.01%
39	Hexane	110-54-3	alkane	0.016	0.9998	2.83%
40	1,1-Dichloroethane	75-34-3	Halogenated hydrocarbons	0.031	0.9999	3.68%
41	Vinyl acetate	108-05-4	OVOCs	0.015	0.9998	3.20%
42	2,4-Dimethylpentane	108-08-7	alkane	0.007	0.9975	3.45%
43	Methylcyclopentane	96-37-7	alkane	0.015	0.9976	3.53%

44	Trans-1,2-dichloroethylene	156-60-5	Halogenated hydrocarbons	0.02	0.9997	4.04%
45	cis-1,2-Dichloroethylene	156-59-2	Halogenated hydrocarbons	0.024	0.9998	3.31%
46	2-Butanone	78-93-3	OVOCs	0.05	0.9965	4.29%
47	ethyl acetate	141-78-6	OVOCs	0.029	0.9971	4.91%
48	Tetrahydrofuran	109-99-9	OVOCs	0.022	0.9996	3.57%
49	trichloromethane	67-66-3	Halogenated hydrocarbons	0.029	0.9997	4.34%
50	1,1,1-Trichloroethane	71-55-6	Halogenated hydrocarbons	0.027	0.9998	3.61%
51	2-Methylhexane	591-76-4	alkane	0.011	0.9975	3.50%
52	Cyclohexane	110-82-7	alkane	0.02	0.9998	3.04%
53	2,3-Dimethylpentane	565-59-3	alkane	0.007	0.9977	3.16%
54	carbon tetrachloride	56-23-5	Halogenated hydrocarbons	0.024	0.9998	3.42%
55	3-Methylhexane	589-34-4	alkane	0.016	0.9976	4.10%
56	benzene	71-43-2	Aromatic hydrocarbons	0.018	0.9999	3.21%
57	1,2-Dichloroethane	107-06-2	Halogenated hydrocarbons	0.027	0.9997	3.43%
58	2,2,4-Trimethylpentane	540-84-1	alkane	0.015	0.9977	3.17%
59	Heptane	142-82-5	alkane	0.009	0.9997	3.12%
60	trichloroethylene	79-01-6	Halogenated hydrocarbons	0.02	0.9997	3.40%
61	Methylcyclohexane	108-87-2	alkane	0.011	0.9978	2.63%
62	1,2-Dichloropropane	78-87-5	Halogenated hydrocarbons	0.018	0.9999	3.56%
63	Methyl methacrylate	80-62-6	OVOCs	0.029	0.9992	1.87%
64	1,4-Dioxane	123-91-1	OVOCs	0.05	0.9992	3.26%
65	Dichloromethane	75-27-4	Halogenated hydrocarbons	0.024	0.9985	2.94%

66	2,3,4-Trimethylpentane	565-75-3	alkane	0.009	0.9975	2.70%
67	2-Methylheptane	592-27-8	alkane	0.016	0.9974	2.40%
68	Trans-1,3-dichloropropene	10061-02-6	Halogenated hydrocarbons	0.018	0.9998	3.71%
69	3-Methylheptane	589-81-1	alkane	0.013	0.9979	2.44%
70	Methyl isobutyl ketone	108-10-1	OVOCs	0.05	0.9992	3.35%
71	toluene	108-88-3	Aromatic hydrocarbons	0.011	0.9993	2.74%
72	n-octane	111-65-9	alkane	0.016	0.9979	2.50%
73	cis-1,3-dichloropropene	10061-01-5	Halogenated hydrocarbons	0.007	0.9997	2.26%
74	1,1,2-Trichloroethane	79-00-5	Halogenated hydrocarbons	0.026	0.9996	2.56%
75	tetrachloroethylene	127-18-4	Halogenated hydrocarbons	0.026	0.9997	2.82%
76	2-Hexanone	591-78-6	OVOCs	0.05	0.9992	3.13%
77	Dibromochloromethane	124-48-1	Halogenated hydrocarbons	0.015	0.9966	2.67%
78	1,2-Dibromoethane	106-93-4	Halogenated hydrocarbons	0.018	0.9998	2.62%
79	chlorobenzene	108-90-7	Halogenated hydrocarbons	0.011	0.9997	2.16%
80	ethylbenzene	100-41-4	Aromatic hydrocarbons	0.009	0.9997	1.23%
81	m-Xylene	108-38-3	Aromatic hydrocarbons	0.022	0.9996	1.07%
82	Paraxylene	106-42-3	Aromatic hydrocarbons	0.022	0.9996	1.07%
83	Nonane	111-84-2	alkane	0.022	0.9979	1.15%
84	o-xylene	95-47-6	Aromatic hydrocarbons	0.015	0.9996	1.32%
85	styrene	100-42-5	Aromatic hydrocarbons	0.018	0.9994	1.07%
86	Bromoform	75-25-2	Halogenated hydrocarbons	0.022	0.9957	1.84%
87	Cumene	98-82-8	Aromatic hydrocarbons	0.013	0.9983	1.31%

88	1,1,2,2-Tetrachloroethane	79-34-5	Halogenated hydrocarbons	0.018	0.9993	1.87%
89	Propylene	103-65-1	Aromatic hydrocarbons	0.026	0.9983	2.31%
90	m-Ethyltoluene	620-14-4	Aromatic hydrocarbons	0.038	0.999	2.58%
91	4-Ethyltoluene	622-96-8	Aromatic hydrocarbons	0.027	0.999	1.46%
92	1,3,5-Trimethylbenzene	108-67-8	Aromatic hydrocarbons	0.007	0.9992	1.84%
93	decane	124-18-5	alkane	0.038	0.9981	2.50%
94	2-Ethyltoluene	611-14-3	Aromatic hydrocarbons	0.022	0.9986	2.33%
95	1,2,4-Trimethylbenzene	95-63-6	Aromatic hydrocarbons	0.007	0.9978	2.52%
96	1,3-Dichlorobenzene	541-73-1	Halogenated hydrocarbons	0.016	0.9978	3.70%
97	1,4-Dichlorobenzene	106-46-7	Halogenated hydrocarbons	0.024	0.997	4.56%
98	1,2,3-Trimethylbenzene	526-73-8	Aromatic hydrocarbons	0.035	0.9982	2.93%
99	Benzyl chloride	100-44-7	Halogenated hydrocarbons	0.013	0.9976	3.30%
100	m-Diethylbenzene	141-93-5	Aromatic hydrocarbons	0.04	0.9964	3.09%
101	p-Diethylbenzene	105-05-5	Aromatic hydrocarbons	0.04	0.9945	3.88%
102	1,2-Dichlorobenzene	95-50-1	Halogenated hydrocarbons	0.007	0.9979	1.69%
103	Undecane	1120-21-4	alkane	0.033	0.9942	4.58%
104	Dodecane	112-40-3	alkane	0.05	0.9942	4.21%
105	1,2,4-Trichlorobenzene	120-82-1	Halogenated hydrocarbons	0.046	0.997	4.36%
106	Hexachloro-1,3-butadiene	87-68-3	Halogenated hydrocarbons	0.007	0.9965	2.84%
107	naphthalene	91-20-3	Aromatic hydrocarbons	0.022	0.9903	3.25%

Table S1. Summary of details of VOCs analysis.

Briefly, the signal-noise balance is given by the following equation:

$$Noise = \sqrt{\frac{\sum_{i=m}^{m+n} (x_i - \bar{x})^2}{n+1}} \dots\dots\dots (S1)$$

$$SNR(dB) = 20 * \text{Log}_{10}(SNR) \dots\dots\dots (S2)$$

Where

SNR: signal-to-noise ratio;

Signal: the peak signal after deducting the background baseline;

m: the starting point for calculating the background baseline;

m+n: the endpoint of the calculation background baseline;

- is the data value;

- is the average of the data for this segment, which is the background baseline value

SNR(dB) – Signal-to-Noise Ratio (dB)