

Supplementary Materials: The Impact of Anthropogenic VOC Emissions on Atmospheric Pollution: A Case Study of a Typical Industrialized Area in China

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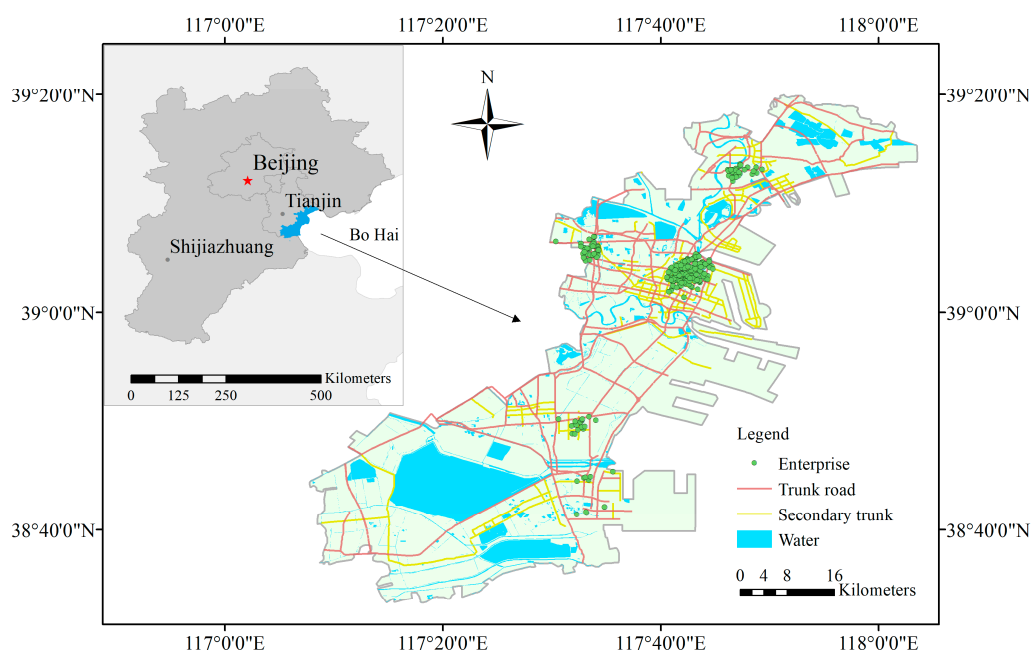


Figure S1. Study area.

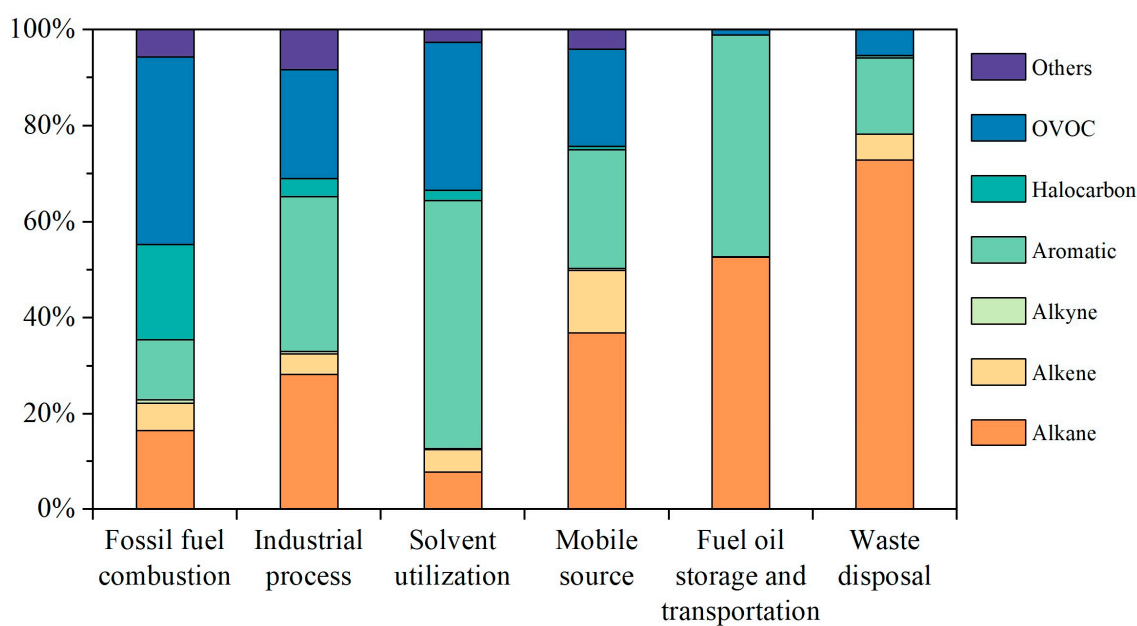


Figure S2. Composition of VOCs in emission sources.

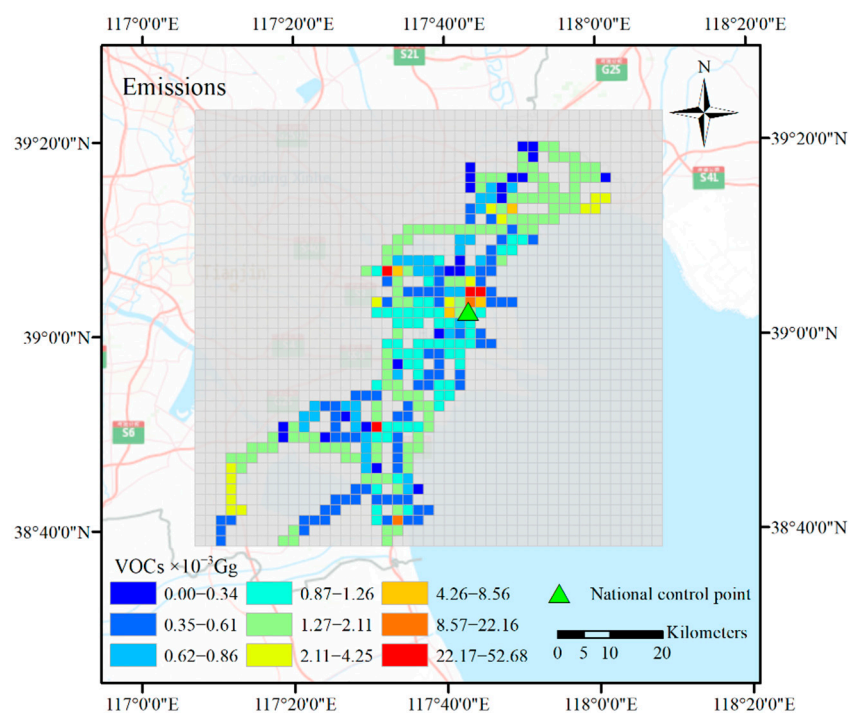


Figure S3. VOC emissions spatial distribution.

(As model input file)

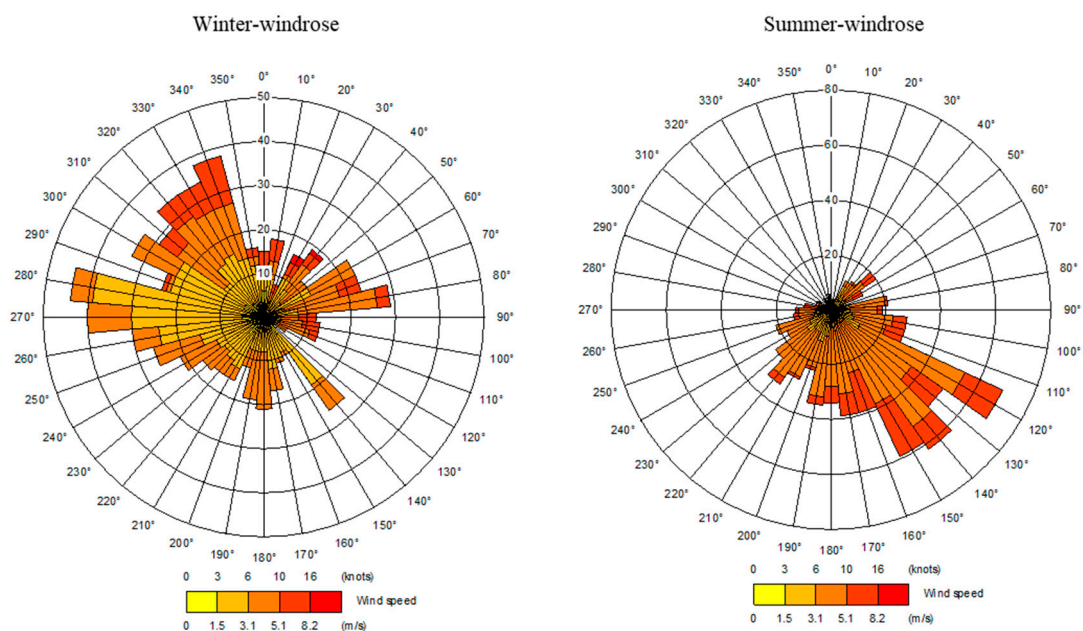


Figure S4. Windrose.

Table S1. Source classification and emission factors.

Level 1	Level 2	Level 3	Emission factor	Unit	Ref.
Number	Sub-source				
Stationary fossil fuel	1	Power generation	Coal	0.04	g/kg
			Natural gas	0.02	g/m ³
	2	Thermal	Coal	0.04	g/kg

(HE
K.2015)

Level 1	Level 2	Level 3	Emission factor	Unit	Ref.
Number	Sub-source				
combustion	3	Industrial combustion	Fuel oil	2.88	g/kg
			Natural gas	0.12	g/m ³
	4	Non-metal mineral product	Glass/ceramic	4.40/29.22	g/kg
			Wood-based panel	0.5	g/m ³
	5	Petroleum processing and coking industry	Coke/crude oil production/processing/refining	2.96/1.42/0.32/1.82	g/kg
			Polyvinyl chloride/polystyrene/high-density polyethylene/polypropylene/urea/compound fertilizer/ink/dye/architectural paint/adhesive	0.74/5.40/5.70/3/0.01/0/5/81.40/15/20	g/kg
Industrial process	7	Rubber and plastic manufacturing	Foam/faux leather	770/0.18	g/kg
			Tires	0.91	kg/ piece
	8	Wine production	Alcohol/beer/wine/liquor	218.25/0.25/0.50/25	g/kg
	9	Food production	Bread/pastries/biscuits/bacon	10.62/1/1/0.14	g/kg
	10	Agricultural and sideline food processing	Sugar/corn oil/peanut oil/soybean oil	8/9.35/10.35/2.45	g/kg
	11	Other industrial processes	Polyester/nylon/pulp/silk/cloth	0.7/3.30/3.10/10/10	g/kg
Solvent utilization	12	Printing and dyeing	Traditional ink printing/New ink printing/dye printing	750/100/81.40	g/kg
			Waterborne architectural coatings/solvent-based architectural coatings/Wood furniture coating	120/450/640	g/kg
			Car painting/bicycle painting/motorcycle painting	21.20/0.30/1.80	kg/ vehicle
	13	Surface coating	Metal furniture coating/home appliance coating/equipment manufacturing coating	0.20/0.20/0.40	kg/ piece
			Wood production	0.22	g/m ³
			Adhesive use	85	g/kg
Mobile source	14	Other utilization	Office supplies	25	t/ factory/year
Storage and transportation	15/16/17/18/19	Light-duty gasoline vehicles/heavy-duty gasoline vehicles/light-duty diesel trucks/heavy-duty diesel trucks/motorcycles			(MEE,2014)
Waste disposal	20	Gas station	Gasoline	3.24	g/kg
	21		Diesel	0.08	g/kg
	22	Solid waste treatment	Garbage	0.74	g/kg

Table S2. VOC Species MIR and OFP ($\times 10^{-3}$ Gg).

	Chemical groups	Species name	CAS	MIR	OFP($\times 10^{-3}$ Gg)
1	Alkane	Ethane	74-84-0	0.321	10.05
2	Alkane	Propane	74-98-6	0.563	13.82
3	Alkane	i-Butane	75-28-5	1.300	13.57
4	Alkane	n-Butane	106-97-8	1.330	22.85
5	Alkane	Cyclopentane	287-92-3	2.370	4.66
6	Alkane	i-Pentane	78-78-4	1.650	99.34
7	Alkane	n-Pentane	109-66-0	1.560	33.78
8	Alkane	Methylcyclopentane	96-37-7	2.230	14.33
9	Alkane	Cyclohexane	110-82-7	1.810	65.48
10	Alkane	2,2-Dimethylbutane	75-83-2	1.300	4.67
11	Alkane	2,3-Dimethylbutane	79-29-8	1.090	7.03
12	Alkane	2-Methylpentane	107-83-5	1.770	37.05
13	Alkane	3-Methylpentane	96-14-0	2.090	39.25
14	Alkane	n-Hexane	110-54-3	1.550	92.89
15	Alkane	n-Heptane	142-82-5	1.370	14.05
16	Alkane	Isoheptane	591-76-4	1.570	11.63
17	Alkane	3-Methylhexane	589-34-4	1.910	14.71
18	Alkane	2,3-Dimethylpentane	565-59-3	1.550	5.64
19	Alkane	2,4-Dimethylpentane	108-08-7	1.760	11.40
20	Alkane	Ethylcyclohexane	1678-91-7	1.820	0.23
21	Alkane	2,2,4-Trimethylpentane	540-84-1	1.380	15.40
22	Alkane	2,3,4-Trimethylpentane	565-75-3	1.200	5.59
23	Alkane	2-Methylheptane	592-27-8	1.370	4.31
24	Alkane	3-Methylheptane	589-81-1	1.530	5.54
25	Alkane	Methylcyclohexane	108-87-2	1.860	14.72
26	Alkane	n-Octane	111-65-9	1.150	7.85
27	Alkane	n-Nonane	111-84-2	1.030	6.53
28	Alkane	n-Decane	124-18-5	0.926	15.28
29	Alkane	n-Undecane	1120-21-4	0.849	19.44
30	Alkane	n-Dodecane	112-40-3	0.785	26.36
31	Alkene	Ethene	74-85-1	8.640	353.62
32	Alkene	Propene	115-07-1	10.800	333.11
33	Alkene	1,3-Butadiene	106-99-0	11.500	87.43
34	Alkene	1-Butene	106-98-9	9.300	179.49
35	Alkene	i-butene	115-11-7	5.370	15.40
36	Alkene	cis-2-Butene	590-18-1	12.200	35.10
37	Alkene	trans-2-Butene	624-64-6	12.500	47.06
38	Alkene	Isoprene	78-79-5	9.710	5.51
39	Alkene	1-Pentene	109-67-1	6.920	20.71
40	Alkene	cis-2-Pentene	627-20-3	9.620	9.58
41	Others	Acrylonitrile	107-13-1	2.210	20.18
42	Alkene	trans-2-Pentene	646-04-8	9.740	15.51
43	Alkene	3-Methyl-1-butene	563-45-1	6.750	0.81
44	Alkene	2-Methyl-1-butene	563-46-2	5.740	2.55
45	Alkene	2-Methyl-2-butene	513-35-9	10.400	8.93
46	Alkene	1-Hexene	592-41-6	5.470	33.64
47	Alkene	cis-2-Hexene	7688-21-3	7.760	0.97
48	Alkene	2-Methyl-1-pentene	763-29-1	4.730	0.97
49	Alkyne	Ethyne	74-86-2	0.944	4.39

	Chemical groups	Species name	CAS	MIR	OFP($\times 10^{-3}$ Gg)
50	Aromatic	Benzene	71-43-2	0.787	36.93
51	Aromatic	Toluene	108-88-3	4.020	383.29
52	Aromatic	Ethylbenzene	100-41-4	3.110	209.04
53	Aromatic	o-Xylene	95-47-6	7.170	250.48
54	Aromatic	m/p-Xylene	108-38-3/106-42-3	6.990	453.11
55	Aromatic	Xylene	1330-20-7	7.110	32.25
56	Aromatic	Styrene	100-42-5	1.700	68.98
57	Aromatic	1,2,3-Trimethylbenzene	526-73-8	9.860	121.00
58	Aromatic	1,2,4-Trimethylbenzene	95-63-6	7.880	262.56
59	Aromatic	1,3,5-Trimethylbenzene	108-67-8	9.350	112.33
60	Aromatic	n-Propylbenzene	103-65-1	2.150	10.73
61	Aromatic	Isopropylbenzene	98-82-8	2.580	9.12
62	Aromatic	o-Ethyltoluene	611-14-3	5.330	60.70
63	Aromatic	m-Ethyltoluene	620-14-4	6.700	176.29
64	Aromatic	p-Ethyltoluene	622-96-8	4.280	44.06
65	Aromatic	o-Diethylbenzene	135-01-3	5.140	2.04
66	Aromatic	m-Diethylbenzene	141-93-5	6.300	16.38
67	Aromatic	p-Diethylbenzene	105-05-5	4.180	18.18
68	Aromatic	1-Methyl-3-propylbenzene	1074-43-7	6.300	1.55
69	Aromatic	1-Methyl-4-propylbenzene	1074-55-1	4.180	0.49
70	Aromatic	2-Ethyl-1,4-dimethyl-benzene	1758-88-9	6.720	3.30
71	Aromatic	1-Ethyl-2,4-dimethylbenzene	874-41-9	6.720	1.82
72	Aromatic	Naphthalene	91-20-3	3.130	11.40
73	Halocarbon	Chloroform	67-66-3	0.026	0.06
74	Halocarbon	Dichloromethane	75-09-2	0.049	0.42
75	Halocarbon	Chloromethane	74-87-3	0.042	0.06
76	Halocarbon	Methyl bromide	74-83-9	0.021	0.01
77	Halocarbon	Tetrachloroethylene	127-18-4	0.037	0.07
78	Halocarbon	Trichloroethylene	79-01-6	0.746	0.34
79	Halocarbon	1,1-Dichloroethylene	75-35-4	2.080	0.22
80	Halocarbon	1,1,1-Trichloroethane	71-55-6	0.005	0.00
81	Halocarbon	Vinyl chloride	75-01-4	3.190	9.06
82	Halocarbon	1,1,2-Trichloroethane	79-00-5	0.094	0.97
83	Halocarbon	1,1-Dichloroethane	75-34-3	0.084	0.01
84	Halocarbon	1,2-Dichloroethane	107-06-2	0.228	1.36
85	Halocarbon	Chloroethane	75-00-3	0.343	0.19
86	Halocarbon	cis-1,3-Dichloropropene	10061-01-5	3.660	1.49
87	Halocarbon	trans-1,3-Dichloropropene	10061-02-6	4.730	15.13
88	Halocarbon	1,2-Dichloropropane	78-87-5	0.319	0.43
89	Halocarbon	1,2-Dichlorobenzene	95-50-1	0.197	0.08
90	Halocarbon	1,4-Dichlorobenzene	106-46-7	0.197	0.12
91	Halocarbon	Chlorobenzene	108-90-7	0.351	0.52
92	Halocarbon	Dibromoethane	106-93-4	0.108	0.03
93	Halocarbon	Trans-1,2-Dichloroethylene	156-60-5	1.800	0.28
94	OVOC	Methanol	67-56-1	0.668	6.39
95	OVOC	Ethanol	64-17-5	1.790	54.39
96	OVOC	Ethylene glycol	107-21-1	3.400	14.26
97	OVOC	Propylene glycol	57-55-6	2.470	3.31
98	OVOC	Isopropanol	67-63-0	0.644	12.38

	Chemical groups	Species name	CAS	MIR	OFP($\times 10^{-3}$ Gg)
99	OVOC	n-Butanol	71-36-3	3.270	20.88
100	OVOC	Diethylene glycol	111-46-6	3.960	3.84
101	OVOC	2-Ethyl-1-hexanol	104-76-7	2.290	0.35
102	OVOC	2-Methyl-2-propanol	75-65-0	0.424	0.34
103	OVOC	Isobutanol	78-83-1	2.750	0.34
104	OVOC	Formaldehyde	50-00-0	7.160	379.33
105	OVOC	Acetaldehyde	75-07-0	6.070	47.62
106	OVOC	Acrolein	107-02-8	6.980	31.41
107	OVOC	Propionaldehyde/Propanal	123-38-6	6.780	31.49
108	OVOC	Crotonaldehyde	4170-30-3	8.180	2.90
109	OVOC	Methacrolein	78-85-3	5.430	14.92
110	OVOC	Isovaleraldehyde	590-86-3	4.690	7.18
111	OVOC	Heptaldehyde	111-71-7	3.550	15.19
112	OVOC	Octanal	124-13-0	3.060	3.19
113	OVOC	o-Tolualdehyde	529-20-4	-0.29	-0.09
114	OVOC	2,5-Dimethylbenzaldehyde	5779-94-2	-0.26	-0.81
115	OVOC	Tolualdehyde	1334-78-7	-0.29	-0.94
116	OVOC	Acetone	67-64-1	0.343	24.82
117	OVOC	Methylethylketone	78-93-3	1.530	43.78
118	OVOC	Diacetyl	431-03-8	13.500	8.30
119	OVOC	2-pentanone	107-87-9	3.060	1.75
120	OVOC	3-Pentanone	96-22-0	1.430	0.14
121	OVOC	Cyclohexanone	108-94-1	1.660	2.64
122	OVOC	4-Methyl-2-Pentanone	108-10-1	3.810	60.31
123	OVOC	Methyl Vinyl ketone	78-94-4	9.060	8.33
124	OVOC	Methyl n-butyl ketone	563-80-4	1.780	0.30
125	OVOC	2-Hexanone	591-78-6	3.470	3.28
126	OVOC	Methyl acetate	79-20-9	0.079	0.11
127	OVOC	Vinyl acetate	108-05-4	2.870	60.39
128	OVOC	Ethyl acetate	141-78-6	0.721	32.14
129	OVOC	Methyl methacrylate	80-62-6	11.700	17.99
130	OVOC	1-Methoxy-2-propylacetate	108-65-6	1.790	9.94
131	OVOC	Isobutyl acetate	110-19-0	0.695	0.10
132	OVOC	sec-Butyl acetate	105-46-4	1.510	18.73
133	OVOC	Carbonic acid , dimethyl ester	616-38-6	0.065	0.01
134	OVOC	Aceticacid,1-methylethylester	108-21-4	1.100	0.11
135	OVOC	2-Pentanol,acetate	628-63-7	1.180	0.14
136	OVOC	MTBE/methyl tertiary butyl ether	1634-04-4	0.785	4.58
137	OVOC	2-Butoxyethanol	111-76-2	3.000	7.21
138	OVOC	1,4-Dioxane	123-91-1	2.680	5.57
139	OVOC	Dimethoxymethane	109-87-5	1.490	2.05
140	OVOC	Tetrahydrofuran	109-99-9	4.770	19.99

Table S3. VOC Species Y_{SOA} and SOAP (%).

	Chemical groups	Species	CAS	Avg. Y_{SOA} (%)	SOAP (%)
1	Aromatic	1,2,4-trimethylbenzene	95-63-6	2.01	0.78
2	Aromatic	m/p-xylene	108-38-3/ 106-42-3	7.05	5.32
3	Alkane	n-undecane	1120-21-4	33	8.79
4	Alkane	methylcyclohexane	108-87-2	22	2.03

	Chemical groups	Species	CAS	Avg. Y _{SOA} (%)	SOAP (%)
5	Aromatic	o-ethyltoluene	611-14-3	5.6	0.74
6	Aromatic	1,3,5-trimethylbenzene	108-67-8	2.1	0.29
7	Aromatic	p-ethyltoluene	622-96-8	2.5	0.30
8	Aromatic	p-diethylbenzene	105-05-5	6.3	0.32
9	Alkane	2,2,4-trimethylpentane	540-84-1	4.8	0.62
10	Alkane	2-methylheptane	592-27-8	4.8	0.18
11	OVOC	MTBE/methyl tertiary butyl ether	1634-04-4	0.1	0.01
12	OVOC	methylethylketone	78-93-3	0.78	0.26
13	Aromatic	n-propylbenzene	103-65-1	1.6	0.09
14	OVOC	4-methyl-2-pentanone	108-10-1	0.78	0.14
15	Aromatic	o-xylene	95-47-6	10	4.06
16	Alkane	cyclohexane	110-82-7	0.17	0.07
17	Alkane	methylcyclopentane	96-37-7	0.17	0.01
18	Aromatic	Isopropylbenzene	98-82-8	4	0.16
19	Alkane	n-nonane	111-84-2	13	1.03
20	Alkene	isoprene	78-79-5	0.79	0.01
21	Alkane	n-heptane	142-82-5	4.8	0.57
22	Alkene	1-hexene	592-41-6	2	0.14
23	Alkane	n-octane	111-65-9	5.8	0.46
24	Alkane	cyclopentane	287-92-3	4	0.09
25	Alkane	n-dodecane	112-40-3	44	17.19
26	Alkene	1,3-butadiene	106-99-0	13	1.15
27	Aromatic	m-diethylbenzene	141-93-5	6.3	0.19
28	Aromatic	m-ethyltoluene	620-14-4	6.3	1.93
29	Aromatic	styrene	100-42-5	3.9	1.84
30	Alkane	2,3,4-trimethylpentane	565-75-3	4.8	0.26
31	OVOC	heptaldehyde	111-71-7	9.3	0.46
32	OVOC	methyl vinyl ketone	78-94-4	0.78	0.01
33	OVOC	acetone	67-64-1	0.78	0.66
34	OVOC	octanal	124-13-0	9.3	0.11
35	OVOC	isovaleraldehyde	590-86-3	9.3	0.17
36	Halocarbon	chlorobenzene	108-90-7	5.4	0.09
37	Halocarbon	1,4-dichlorobenzene	106-46-7	1.6	0.01
38	Aromatic	benzene	71-43-2	0.93	0.51
39	Aromatic	toluene	108-88-3	36	39.93
40	Halocarbon	1,3-dichlorobenzene	541-73-1	1.6	0.01
41	Aromatic	ethylbenzene	100-41-4	5.4	4.22
42	Halocarbon	1,2-dichlorobenzene	95-50-1	1.6	0.01
43	Aromatic	o-diethylbenzene	135-01-3	6.3	0.03
44	Alkane	n-decane	124-18-5	22	4.22
45	OVOC	2-pentanone	107-87-9	0.78	0.01
46	Aromatic	1,2,3-trimethylbenzene	526-73-8	2.1	0.30
47	OVOC	3-pentanone	96-22-0	0.78	0.00
48	Alkane	3-methylheptane	589-81-1	4.8	0.20