Supplement of

Characteristics of VOCs and their potentials for O₃ and SOA formation in a medium-sized city in eastern China

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**Table S1.** Species of VOCs measured in this study

| Categories (a)                        | Species                                                                 |
|---------------------------------------|-------------------------------------------------------------------------|
| Alkanes (29 species)                  | Ethane; Propane; N-butane; Isobutane; N-pentane; 1-Pentene; N-octane; N-  |
|                                       | nonane; N-decane; N-undecane; N-dodecane; Isopentane; Cyclopentane; N-  |
|                                       | hexane; Cyclohexane; Heptane; 2-Methylheptane; Methylcyclohexane; 3-     |
|                                       | Methylheptane; 2-Methylhexane; 3-Methylhexane; 2,2-Dimethylbutane; 2,3-  |
|                                       | Dimethylbutane; 2-Methyl pentane; 3-Methyl pentane; 2,3-Dimethylpentane;|
|                                       | 2,2,4-Trimethylpentane; 2,3,4-Trimethylpentane; 2,4-Dimethylpentane      |
| Alkenes (12 species)                  | Ethylene; Propylene; 1-Butene; Cis-2-butene; Trans-2-butene; 1,3-Butadiene; |
|                                       | Methylcyclopentane; Cis-2-pentene; Trans-2-pentene; Isoprene; 1-Hexene;  |
|                                       | Acetylene                                                               |
| Aromatic hydrocarbons (17 species)    | Benzene; Toluene; O-xylene; M/p-xylene; N-propylbenzene; Cumene;        |
|                                       | Styrene; Naphthalene; Ethylbenzene; 2-Ethyltoluene; 3-Ethyltoluene; 4-  |
|                                       | Ethyltoluene; 1,3-Diethylbenzene; 1,4-Diethylbenzene; 1,2,3-            |
|                                       | Trimethylbenzene; 1,2,4-Trimethylbenzene; 1,3,5-Trimethylbenzene         |
| Halohydrocarbons (35 species)         | Freon 11; Freon 12; Freon 113; Freon 114; Methyl bromide;               |
|                                       | Dichloromethane; Chlorobenzene; Tetrachloroethylene; Trichloroethylene; |
|                                       | Benzyl chloride; Chloroform; Chloroethane; Bromoform; Methyl chloride;  |
|                                       | 1,2-Dichloroethane; 1,2-Dibromoethane; 1,1-Dichloroethane; Vinyl chloride; |
|                                       | 1,2-Dichloropropane; Dichlorodibromomethane; 1,1,1-Trichloroethane;     |
|                                       | 1,1,2,2-Tetrachloroethane; Dichlorobromomethane; 1,2,4-Trichlorobenzene;|
|                                       | 1,4-Dichlorobenzene; 1,3-Dichlorobenzene; 1,1-Dichloroethylene; Cis-1,2-|
|                                       | dichloroethylene; Trans-1,2-dichloroethylene; O-dichlorobenzene; 1,1,2-|
|                                       | Trichloroethane; Trans-1,3-dichloro-1-propene; Cis-1,3-dichloropropene;|
|                                       | Carbon tetrachloride; Hexachloro-1,3-butadiene                           |
| OVOCs (13 species)                    | Ethanol; Acrolein; Acetone; Isopropanol; 1,4-Dioxane; Ethyl acetate;    |
|                                       | Vinyl acetate; 2-Butanone; Tetrahydrofuran; 4-Methyl-2-pentanone; Methyl tert |
|                                       | butyl ether; Methyl methacrylate; Methyl n-butyl ketone                  |

Notes: (a) the automatic measurements include all the 106 species of VOCs, and the manual measurements include the 56 PAMS species of NMHCs (alkanes, alkenes and aromatic hydrocarbons); (b) acetylene was included here.
Table S2. Top ten species of the NMHCs-56 along with their concentrations (Conc, ppbv) and proportions (Prop, %) at the three sites based on manual measurements.

| Rank | HMS | Species | Conc/Prop | CMS | Species | Conc/Prop | HNU | Species | Conc/Prop |
|------|-----|---------|-----------|-----|---------|-----------|-----|---------|-----------|
|      |     | Species | Conc/Prop |     | Species | Conc/Prop |     | Species | Conc/Prop |
| 1    |     | Propane | 2.89 / 19.38 |     | Propane | 6.17 / 27.60 |     | Propane | 3.16 / 13.09 |
| 2    |     | Ethane  | 2.23 / 14.96 |     | Ethane  | 2.46 / 11.02 |     | Toluene | 2.70 / 11.18 |
| 3    |     | Acetylene | 1.53 / 10.26 |     | Toluene | 2.24 / 10.04 |     | Ethane  | 2.63 / 10.89 |
| 4    |     | N-butane | 1.31 / 8.76  |     | Ethylene | 1.86 / 8.32  |     | M/p-xylene | 2.25 / 9.32 |
| 5    |     | Isobutane | 1.28 / 8.56  |     | Isobutane | 1.60 / 7.16  |     | Isobutane | 1.99 / 8.27 |
| 6    |     | Ethylene | 1.05 / 7.04  |     | Acetylene | 1.43 / 6.38  |     | Ethylene | 1.99 / 8.25 |
| 7    |     | N-hexane | 1.01 / 6.80  |     | N-butane | 1.06 / 4.74  |     | Acetylene | 1.85 / 7.66 |
| 8    |     | Toluene  | 0.82 / 5.51  |     | M/p-xylene | 1.05 / 4.68  |     | 1-Butene | 1.38 / 5.70 |
| 9    |     | M/p-xylene | 0.50 / 3.32  |     | N-hexane | 0.72 / 3.21  |     | N-hexane | 1.06 / 4.41 |
| 10   |     | Benzene  | 0.36 / 2.41  |     | 1-Butene | 0.66 / 2.94  |     | N-butane | 1.01 / 4.21 |
| SUM  |     | --       | 12.97 / 87.00 |     | --       | 19.25 / 86.08 |     | --       | 20.01 / 82.98 |
Fig. S1. Comparison on total concentration of the NHMCs between manual and automatic measurements with standard deviations.
Fig. S2. Factor profiles obtained by the PMF model at the three sites of (a) HMS, (b) CMS, and (c) HNU.

Notes:

(1) Vehicle emission refers to the emissions of motor vehicles fueled by diesel, gasoline, and LPG, which mainly emit alkanes with carbon atom number less than 6, such as ethane, propane, ethylene, and isopentane, as well as some aromatics and alkenes (Liu et al., 2016; Marinello et al., 2020).
(2) Solvent usage usually refers to solvent application in printing, spraying and industrial process, which mainly emit aromatic hydrocarbons, such as toluene, xylene, ethylbenzene, styrene, trimethylbenzene, n-propyl benzene, and ethyltoluene (He et al., 2019; Song et al., 2019).

(3) Industrial process includes many kinds of industrial activities such as oil refining, chemical manufacturing, and food manufacturing. The emissions usually include a variety of alkanes, alkenes, and aromatics (Wei et al., 2018; Hui et al., 2020).

(4) Gas evaporation refers to the volatilization and leakage of diesel, gasoline, and LPG during storage and transportation, which mainly emits isopentane, n-pentane, ethane and propane (Liu et al., 2016; Ma et al., 2019).

(5) Biomass burning refers to straw and firewood combustion, and the main VOC species of emissions include methyl chloride, acetonitrile, ethylene, and propylene (Yang et al., 2021).

(6) Fossil fuel combustion refers to the combustion of fossil fuels such as coal and natural gas, and its typical species of VOCs are mainly acetylene and a small amount of alkanes and aromatics (Zhou et al., 2019; Sha et al., 2021).

(7) Biogenic emission refers to emissions of plants, and the typical species of VOCs are isoprene and terpenes (Sha et al., 2021).
Fig. S3. Monthly OFPs and proportions (marked on the bars) of different VOC categories at the three sites.

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