Data of chemical composition of the particles from OH-initiated oxidation of 1,3,5-trimethylbenzene

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**A R T I C L E   I N F O**

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**A B S T R A C T**

This paper presents the data of chemical composition of the particles from OH oxidation reaction of 1,3,5-trimethylbenzene (1,3,5-TMB). The particle-phase compositions are measured on-line by using a vacuum ultraviolet (VUV) photoionization aerosol mass spectrometer. The assignments of the major peaks of photoionization mass spectrum, as well as their molecular structures, are presented. The optimized structures of the reactants, intermediates and transition states involved in the reaction of the bicyclic peroxy radical with HO\textsubscript{2} are shown. The reaction routes of the OH-initiated oxidation of the deuterated 1,3,5-TMB sample are also calculated and displayed for comparison. The data presented here is related to the paper “Direct observation of the particle-phase bicyclic products from OH-initiated oxidation of 1,3,5-trimethylbenzene under NOx-free conditions” by Lin et al. (2022).

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Specifications Table

| Subject            | Chemistry            |
|--------------------|----------------------|
| Specific subject area | Atmospheric chemistry |
| Type of data       | Table                |
|                     | Figure               |
|                     | Graph                |
| How the data were acquired | Mass spectra: Vacuum ultraviolet (VUV) photoionization aerosol mass spectrometer. Structures and reaction routes: ChemBioDraw Ultra 12.0, Gaussian 16 and GaussView 6. |
| Data format        | Raw                  |
|                     | Analysed             |
|                     | Filtered             |
| Description of data collection | The mass spectra of the particle-phase products from OH oxidation reaction of 1,3,5-TMB were measured by using the VUV photoionization aerosol mass spectrometer. The molecular structures were drewed manually by using Chemdraw ultra 12.0. The geometric structures were optimized by using Gaussian 16 program. The GaussView as the graphical interface for Gaussian 16 was used to open the output files. |
| Data source location | Institution: Anhui Institute of Optics and Fine Mechanics, CAS City/Town/Region: Hefei, Jinggang, 230031 Country: China |
| Data accessibility | Data are available with this article. The data are also available via ProteomeXchange with the dataset identifier PXD030839. [https://www.ebi.ac.uk/pride/archive/projects/PXD030839](https://www.ebi.ac.uk/pride/archive/projects/PXD030839) |
| Related research article | X. Lin, X. Tang, Z. Wen et al., Direct observation of the particle-phase bicyclic products from OH-initiated oxidation of 1,3,5-trimethylbenzene under NOx-free conditions, Atmospheric Environment. (2022, 271, 118914). [10.1016/j.atmosenv.2021.118914](https://doi.org/10.1016/j.atmosenv.2021.118914) |

Value of the Data

- The data presented in this paper are valuable for the characterization of secondary organic aerosol (SOA) from oxidation of aromatic compounds.
- The data can help researchers to better understand the reaction mechanisms of the bicyclic peroxy radical involved in the atmospheric oxidation.
- The data would serve as a reference for studying or analysing the chemical compositions of SOA from OH-initiated oxidation of 1,3,5-TMB.

1. Data Description

The data of this paper includes one table, two figures and the mass spectrometry raw data open to readers via ProteomeXchange. Concretely, Table 1 lists the molecular structures of the major particle-phase products from OH-initiated oxidation of 1,3,5-trimethylbenzene (1,3,5-TMB). It shows the mass (m/z) and the name of these products and their corresponding molecular structures which were drawn with the ChemBioDraw Ultra program. The oxygen-containing functional groups in these molecular structures are presented in red.
Table 1
The assignments of the particle-phase products from OH-initiated oxidation of 1,3,5-TMB.

| m/z | Product             | Structure                                   | m/z | Product             | Structure                                   |
|-----|---------------------|---------------------------------------------|-----|---------------------|---------------------------------------------|
| 58  | acetone             | ![Acetone structure](image)                 | 130 | citraconic acid     | ![Citraconic acid structure](image)         |
| 60  | acetic acid         | ![Acetic acid structure](image)             |     | mesaconic acid      | ![Mesaconic acid structure](image)          |
| 72  | methyl glyoxal      | ![Methyl glyoxal structure](image)          | 134 | malic acid          | ![Malic acid structure](image)              |
| 74  | hydroxyacetone      | ![Hydroxyacetone structure](image)          | 136 | 2,4,6-trimethyl phenol | ![2,4,6-trimethyl phenol structure](image) |
|     | oxo-acetic acid     | ![Oxo-acetic acid structure](image)         | 138 | 3,5-dimethylphenylhydroperoxide | ![3,5-dimethylphenylhydroperoxide structure](image) |
| 84  | butenedial          | ![Butenedial structure](image)              | 144 | 2-hydroxy-2-methyl-3,4-dioxo-pentanal | ![2-hydroxy-2-methyl-3,4-dioxo-pentanal structure](image) |
| 86  | oxo-propanedioL     | ![Oxo-propanedioL structure](image)         | 150 | 3,5-dimethylbenzoic acid | ![3,5-dimethylbenzoic acid structure](image) |
| 100 | 2,3-dioxobutanal    | ![2,3-dioxobutanal structure](image)       | 152 | (3,5-dimethyl-phenyl)methyl-hydroperoxide | ![3,5-dimethyl-phenyl)methyl-hydroperoxide structure](image) |

(continued on next page)
Table 1 (continued)

| m/z | Product                        | Structure                                      | m/z | Product                        | Structure                                      |
|-----|--------------------------------|------------------------------------------------|-----|--------------------------------|------------------------------------------------|
| 110 | 3-methyl-5-methylidene-5-(2H)furanone | ![Structure](image1)                          | 154 | 4-methyl-hept-4-ene-2,3,6-trione | ![Structure](image2)                          |
| 112 | 2-methyl-4-oxo-2-pentenal         | ![Structure](image3)                          | 156 | 5-hydroxy-4,6-dioxo-2-heptenal  | ![Structure](image4)                          |
|     | 3,5-dimethyl-2(3H)-furanone       | ![Structure](image5)                          | 166 | 3,5-dimethyl-benzenecarboxylic acid | ![Structure](image6)                          |
|     | 3-methyl-2,5-furandione           | ![Structure](image7)                          | 168 | 2-methyl-3-(1-methyl-3-oxobut-1-enyl)-oxirane-2-carbaldehyde | ![Structure](image8)                          |
| 114 | pentane-2,3,4-trione              | ![Structure](image9)                          | 184 | 8-hydroxy-1,3,5-trimethyl-6,7-dioxabicyclo[3.2.1]oct-3-en-2-one | ![Structure](image10)                          |
| 116 | 3-hydroxy-pentane-2,4-dione       | ![Structure](image11)                          | 186 | 1,3,5-trimethyl-6,7-dioxabicyclo[3.2.1]oct-3-ene-2,8-diol | ![Structure](image12)                          |
| 118 | 2-hydroperoxy-2-methylmalonaldehyde | ![Structure](image13)                      | 202 | 8-hydroxy-1,3,5-trimethyl-6,7-dioxabicyclo[3.2.1]oct-3-en-2-hydroperoxide | ![Structure](image14)                          |
| 128 | 2-methyl-4-oxo-pent-2-enoic acid  | ![Structure](image15)                          | 218 | 8-hydroxy-1,3,5-trimethyl-6,7-dioxabicyclo[3.2.1]oct-3-en-2-trioxide | ![Structure](image16)                          |
Fig. 1. Geometric structures of the reactants, intermediates and transition states of the reaction between the O₂-bridged bicyclic peroxy radical (BPR) and HO₂ computed at the M06-2X/MG3S level of theory on the singlet potential energy surfaces.

In addition, Proteome Xchange with the dataset identifier PXD030839 lists the mass spectrometry raw data file (raw data.zip) which can be downloaded publicly. The first two columns of data present the mass (m/z) and the intensity (a.u.) of the mass spectrum from the OH-initiated oxidation of 1,3,5-TMB, and the last two columns show the mass (m/z) and the intensity (a.u.) of the mass spectrum from the OH-initiated oxidation of deuterated 1,3,5-TMB (C₉D₁₂). The corresponding mass spectrum figure file (MS.jpg) can also be seen on-line via the link https://www.ebi.ac.uk/pride/archive/projects/PXD030839.
2. Experimental Design, Materials and Methods

2.1. Materials

1,3,5-TMB (98%) was purchased from Alfa Aesar without further purification, the deuterated 1,3,5-TMB-d12 (98 atom% D) was purchased from Sigma-Aldrich (Saint Louis, MO, USA), and H2O2 (35% in H2O) was obtained from Acros Organics.

2.2. Experimental design

A simulation chamber made of a Teflon bag and surrounded by six ultraviolet lamps (Philips TUV G13 36 W), providing a maximum output at 254 nm, is used to simulate the atmospheric chemical process of OH + 1,3,5-TMB in lab. A home-made vacuum ultraviolet (VUV) photoionization aerosol mass spectrometer (VUV-AMS) is installed to probe and analyze the particle-phase products inside the Teflon bag. A commercial scanning mobility particle sizer (SMPS, TSI 3936, USA) is used to measure the size distribution of the particles. The quantum chemical method using the Gaussian 16 program is adopted to calculate the parameters of the reactants, intermediates and transition states. The configuration of the VUV photoionization aerosol mass spectrometer and the theoretical methods are described in detail in Ref. [1]

2.3. Photoionization mass spectra of the particle-phase products

Raw data of the mass spectra of the particle-phase products from the OH-initiated oxidation reactions of 1,3,5-TMB and deuterated 1,3,5-TMB-d12 (C9D12) measured by using the VUV photoionization aerosol mass spectrometer can be seen in the Supplementary data. A great deal of peaks can be observed in the mass spectrum and most of them have been assigned (see Table 1). The mass spectrometry data have been deposited to the ProteomeXchange Consortium via the PRIDE (Refs. [2,3]) partner repository with the dataset identifier PXD030839.

2.4. The assignments of the main products

The structures of the particle-phase products from the OH-initiated oxidation of 1,3,5-TMB under NOx-free conditions are identified. The main peaks in the VUV photoionization mass spectra have been assigned and listed in Table 1, with the aid of the literature results (Refs. [4,5]). For example, the products of the O2-bridged bicyclic alcohol (m/z = 186) and carbonyl (m/z = 184), the peroxide (m/z = 202) and the trioxide (m/z = 218) products are clearly observed and identified in the particle-phase. In addition, the ring retaining products of 3,5-dimethyl-phenyl-hydroperoxide (m/z = 138), 3,5-dimethylbenzoic acid (m/z = 150), (3,5-dimethyl-phenyl)-methyl-hydroperoxide (m/z = 152), and an array of low mass oxygenated compounds such as acetone, acetic acid and methyl glyoxal are also observed.

2.5. Geometric structures of the main species in the reaction between the BPR radical and HO2

The optimized structures of the reactants, reaction intermediates and transition states involved in the reaction between the O2-bridged bicyclic peroxo radical (BPR) and HO2 on the singlet potential energy surfaces are shown in Fig. 1. The geometric structures were calculated at the M06-2X/MG3S level of theory by using the Gaussian 16 program. The M06-2X functional are hybrid meta density functional theory (DFT) method which has been widely utilized for applications in chemistry (Refs. [6,7]). The selected bond distances such as the hydrogen bond have been given in angstroms.
2.6. Formation mechanism of the deuterated bicyclic oxygenated compounds

The reaction routes of the deuterated 1,3,5-TMB (C₉D₁₂) with OH radical under NOx free conditions are presented in Fig. 2. Similar to the reaction of 1,3,5-TMB with OH, the reaction occurs mainly via the OH addition to form the OH-C₉D₁₂ adduct. In the presence of oxygen, the nascent OH-C₉D₁₂ adduct can react with oxygen to generate the OH-C₉D₁₂-O₂ peroxo radical, which will produce the deuterated bicyclic peroxy radical after subsequent isomerization, reaction with oxygen again and cyclization. Under NOx free condition, reactions of the deuterated bicyclic peroxy radical with the HO₂ radical, other peroxy radicals, and OH radical play a major role. These reactions will produce the deuterated O₂-bridged bicyclic alcohol and carbonyl, the peroxy and the trioxide products. In the self-reaction of the deuterated bicyclic peroxy radical, the deuterium-shift results in the products formation with an odd mass number (m/z = 199 and 195), which are observed in the mass spectrum.

Ethics Statement

The manuscript adheres to ethics in publishing standards.

Appendix A. Supplementary data

Supplementary data to this article can be found online. Raw data of the mass spectra of the particle-phase products from the OH-initiated oxidation reactions of 1,3,5-TMB and deuterated 1,3,5-TMB-d12 (C₉D₁₂).

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

Data of chemical composition of the particles from OH-initiated oxidation of 1,3,5-trimethylbenzene (Original data) (Earth/Chem).

CRediT Author Statement

Xiaoxiao Lin: Investigation, Data curation, Writing – original draft; Xiaofeng Tang: Conceptualization, Methodology, Writing – review & editing, Visualization; Zuoying Wen: Investigation; Bo Long: Investigation, Resources; Christa Fittschen: Investigation; Xuejun Gu: Investigation; Yang Zhang: Investigation; Weijun Zhang: Investigation.

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Supplementary Materials

Supplementary material associated with this article can be found in the online version at doi:10.1016/j.dib.2022.108152.

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