



Linking molecular composition of organic aerosols to reactive oxygen species formation using an MCR-VK framework

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Received: 1 July 2026 – Discussion started: 21 July 2026

Revised: 13 September 2026 – Accepted: 22 September 2026 – Published: 16 October 2026

Abstract. Reactive oxygen species (ROS) formation by atmospheric fine particulate matter (PM) is widely implicated in adverse health effects, yet the molecular determinants of particle-level ROS formation remain poorly constrained, largely due to the chemical complexity of organic aerosol (OA). Here, we link ROS formation to molecular-level OA composition by applying a maximum carbonyl ratio-Van Krevelen framework to ambient fine PM collected from four Chinese megacities, a German semi-urban site, a boreal forest, and laboratory-generated secondary organic aerosol (SOA) from multiple precursors. Using ultrahigh-resolution mass spectrometry combined with hydrogen peroxide (H₂O₂) and radical measurements, we show the intrinsic ROS (H₂O₂ + radicals) formation potential of fine PM is governed by OA composition rather than particle mass. Volume-normalized ROS yields increase with fine PM mass concentration and dominate overall exposure in polluted urban environments. In contrast, mass-normalized ROS yields vary independently of particle loading and are strongly driven by the balance between relative fractions of oxidized organic compounds (RF_{OOC}) and unsaturated organic compounds (RF_{UOC}), i.e., RF_{OOC} / RF_{UOC}. Across urban sites, mass-normalized ROS and H₂O₂ yields exhibit strong correlations with RF_{OOC} / RF_{UOC}, establishing this metric as a robust predictor of ROS formation. Remote, biogenic-influenced aerosols exhibit higher RF_{OOC} / RF_{UOC} and higher ROS yields per unit mass, whereas urban aerosols exhibit the opposite behavior. Laboratory SOA further supports these composition-reactivity relationships, with OOC-rich biogenic SOA exhibiting the highest ROS yields. This study reveals molecular-level characteristics in governing aerosol ROS formation and introduces a framework for assessing health-relevant aerosol oxidative activity of chemically complex OA.

1 Introduction

Exposure to atmospheric fine particulate matter (PM) is linked to a wide range of adverse health outcomes, including respiratory and cardiovascular diseases, and contributes to millions of deaths annually (Burnett et al., 2018; Lelieveld et al., 2015; Zhang et al., 2025; Shiraiwa et al., 2017). A key mechanism underlying these effects is the ability of PM to generate reactive oxygen species (ROS) in biological fluids and cells, triggering oxidative stress, inflammation, and cytotoxicity (Li et al., 2008; Gurgueira et al., 2002; Liu et al., 2022; Lakey et al., 2016). ROS, including hydrogen peroxide (H_2O_2), hydroxyl radicals ($\cdot\text{OH}$), superoxide radicals ($\text{O}_2^{\cdot-}$), and organic radicals, can be produced by a variety of chemically reactive constituents in fine PM, including quinones, transition metals, environmentally persistent free radicals, and secondary organic aerosols (SOA) (Tong et al., 2016; Lin and Yu, 2020; Pöschl and Shiraiwa, 2015; Khachatryan et al., 2011; Yang et al., 2024).

Organic aerosol (OA) components are increasingly recognized as important contributors to the ROS formation of atmospheric aerosols. Multiple field studies have quantified the ROS formation of source-based OA components and demonstrated that OA is a major driver of the ROS formation of ambient fine PM (Zhou et al., 2019; Daellenbach et al., 2020; Liu et al., 2023). Field investigations have also found that some organic species, such as quinone-type compounds, highly oxygenated molecules (HOMs), and organic peroxides, significantly contribute to ROS formation (Verma et al., 2015; Tong et al., 2019, 2021). Complementary laboratory studies have examined the ROS formation of SOA formed from different gaseous precursors under well-controlled conditions (Campbell et al., 2025; Tong et al., 2018; Fang et al., 2024; Liu et al., 2020). These studies show that the oxidative properties of SOA largely depend on precursor identity, reaction conditions, and resulting chemical composition. For example, SOA derived from naphthalene, β -pinene, and isoprene, and have been shown to produce substantial H_2O_2 upon aqueous extraction, with organic hydroperoxides identified as the major ROS contributors (Tong et al., 2018). While these field and laboratory studies highlight the importance of specific OA sources and organic species, most of them have focused on bulk OA characteristics or small sets of target compounds. Consequently, the contributions of individual organic molecules and their structural classes to ROS formation in atmospheric aerosols remain poorly resolved.

This knowledge gap persists largely because atmospheric OA is chemically complex: thousands of species are present, yet only 10%–30% of OA mass is typically identified as specific compounds by the existing analytical techniques (Nozière et al., 2015; Hoffmann et al., 2011). Advances in ultrahigh-resolution mass spectrometry (UHRMS) have substantially expanded molecular-level characterization of OA. Fourier transform ion cyclotron (FT-ICR) and Orbitrap MS

combined with soft ionization techniques including electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI), enable the assignment of thousands of molecular formulas (Zuth et al., 2018; Liu et al., 2025; Wang et al., 2024, 2018a). Molecular metrics such as aromaticity equivalent and double bond equivalent (DBE) are then commonly applied to interpret structural features such as aromaticity and unsaturation (Koch and Dittmar, 2006; Yassine et al., 2014). However, these parameters do not fully capture functional group chemistry that governs redox reactivity.

To overcome this limitation, we recently developed the maximum carbonyl ratio (MCR), a new metric that estimates the maximum number of carbonyl groups a molecule could contain based on its molecular formula (Zhang et al., 2021; Huang et al., 2025). By incorporating MCR into the traditional Van Krevelen (VK) diagram (plots by H/C ratio against O/C ratio) (Ng et al., 2011), we further established an MCR-VK framework that classifies individual compounds into distinct chemical regions. Some of these regions correspond to functional groups or structural features that may be associated with health-related effects. For example, higher MCR values indicate greater carbonyl functionality and electrophilic character, while lower MCR values reflect the dominance of highly oxidized, non-carbonyl species such as (hydro)peroxides, both of which may induce oxidative stress in the respiratory system. As MCR can be easily obtained from UHRMS-assigned formulas, the MCR-VK framework offers a promising new approach to identify organic constituents potentially responsible for ROS formation.

In this study, we apply the MCR-VK framework to investigate the relationship between OA molecular composition and ROS formation by ambient and laboratory-generated aerosols in liquid water (the scheme is illustrated in Fig. S1 in the Supplement). PM samples were collected from urban megacities (Beijing, Xi'an, Shanghai, Guangzhou), a European semi-urban site (Mainz), and a boreal forest site (Hyytiälä), and laboratory-generated SOA was formed from isoprene, monoterpenes, limonene, and naphthalene. Their molecular composition was analyzed using an ultra-high-performance liquid chromatography system coupled with an ESI-Orbitrap mass spectrometer (UHPLC/ESI-Orbitrap-MS). Based on their positions in the MCR-VK diagram, individual molecular formulas were categorized into oxidized organic compounds (OOC) and unsaturated organic compounds (UOC). ROS formation, including both H_2O_2 and radical yields, was quantified. H_2O_2 yields in aerosol aqueous extracts were quantified using a fluorometric probe, and radical yields were measured using electron paramagnetic resonance (EPR) spectroscopy in combination with a spin-trapping method. By integrating molecular-level chemical characterization with ROS measurements, the main objective is to evaluate whether the balance between OOC and UOC can serve as a generalized predictor of ROS formation by atmospheric aerosols. The findings provide a mechanistic basis for understanding OA-driven oxidative stress, offering a

molecularly resolved metric to assess ROS formation by fine PM across diverse environments.

2 Materials and Methods

2.1 Ambient Sample Collection

The ambient PM samples were from six field campaigns, including a boreal-forest station in Hyytiälä, Finland; an urban site in Mainz, Germany; and four Chinese urban sites in Beijing, Xi'an, Shanghai, and Guangzhou. The key sampling details are presented below, while the complete sampling information is shown in Table S1 in the Supplement.

At SMEAR II in Hyytiälä, 47 mm PALL Teflon filters were paired with a Dekati impactor operated at 35 L min^{-1} between 2 and 14 June 2017 (Hari et al., 2012). In Mainz, a model 110-R micro-orifice uniform-deposition impactor (MOUDI; MSP Corporation) was deployed on the roof of the Max Planck Institute for Chemistry from 22 to 30 August 2017. Operating at 30 L min^{-1} , the particles were collected on 47 mm Teflon membranes supplied by Merck Chemicals GmbH (100 nm pore size). In Beijing (Peking University), a TH-16 low-volume (flow rate at 16.7 L min^{-1}) instrument (Tianhong Company, China) was applied for sample collection through 47 mm Whatman® Teflon filters from 26 February 2019 to 10 March 2019. For Xi'an, during 5–9 November 2018, a model TE-20-800 low-pressure cascade impactor (Tisch, USA; $\sim 50 \text{ L min}^{-1}$) was used to collect PM samples through 90 mm Omnipore JVWP09025 Teflon filters (100 nm pore size, Millipore) on the roof of Xi'an Jiaotong University. Shanghai and Guangzhou fine PM samples were collected onto prebaked quartz-fiber filters ($8 \times 10 \text{ in.}$) using a high-volume air sampler (Tisch, Cleveland, OH, USA) at a flow rate of 1050 L min^{-1} from 5 to 27 January 2014.

During each sampling campaign, field blanks were prepared by placing blank filters in the sampler for several minutes without activating the sampling pump. The filters were subsequently retrieved, wrapped in aluminum foil, and stored under the same conditions as the collected samples until analysis. All field blanks were subjected to the same pretreatment and analytical procedures as the particulate matter samples.

2.2 Laboratory SOA generation and Collection

The SOA generation experiments were operated in a 7 L volume quartz flow tube and a 19 L volume potential aerosol mass (PAM) chamber. In the flow tube, particles were formed through gas-phase ozonolysis of α -pinene, β -pinene, or limonene with around 1000 ppb O_3 . In the PAM chamber, isoprene and naphthalene SOA were produced through gas-phase photooxidation under an $\cdot\text{OH}$ concentration of $\sim 5.0 \times 10^{11} \text{ cm}^{-3}$. The concentrations of α -pinene, β -pinene, and limonene were 1–2 ppm, while it was 0.5–1 ppm for isoprene and naphthalene. The generated SOA particle samples were captured onto 47 mm Omnipore Teflon

membrane filters (JVWP04700), which were extracted immediately. The complete information of the SOA generation and sampling is presented in our previous papers (Tong et al., 2018, 2019).

2.3 Ultrahigh Resolution Mass Spectrometer Measurements and Data Processing

The process of sample preparation and instrumental analysis followed established protocols (Zhang et al., 2021; Wang et al., 2018a). Briefly, portions of each filter containing approximately 600 μg of particle mass were extracted two times through ultrasonics for 30 min with 1.5 mL methanol. The two methanolic extracts were pooled and passed through a $0.2 \mu\text{m}$ Teflon syringe membrane to eliminate insoluble residues. After gentle nitrogen evaporation to dryness, the residue was reconstituted in 1.0 mL of a 1 : 9 (*v/v*) acetonitrile–water solution before instrumental analysis.

An UHRMS platform was used for molecular identification. Chromatographic separation was performed on a Dionex UltiMate 3000 UHPLC coupled via a heated electrospray ionization (HESI) source to a Q-Exactive mass spectrometer (Thermo Scientific, Germany). Analytes were resolved with a Hypersil Gold C18 column ($50 \times 2.0 \text{ mm}$; $1.9 \mu\text{m}$ particles; Thermo Scientific, Germany). At 0.5 mL min^{-1} , the binary gradient combined solvent A (ultrapure water containing 2 % acetonitrile and 0.04 % formic acid) with solvent B (acetonitrile containing 2 % ultrapure water). The complete gradient and UHPLC/HESI-Orbitrap settings were adopted from earlier work (Zhang et al., 2021; Zhang, 2023). Data acquisition used negative-ion electrospray (ESI[−]), a resolving power of 70 000 at *m/z* 200, and an *m/z* window of 50–500. The ESI[−] mode preferentially detects polar oxygenated organic compounds and therefore may not capture all organic species in the filter samples. However, all samples were analyzed using the same analytical protocol, enabling consistent comparison of the molecular composition across different ambient environments.

Non-target feature screening was carried out in the open-source package MZmine (v2.37) using the chromatographic and mass-spectral files. Table S2 lists the processing sequence and parameter settings. Signals were considered when peak abundance exceeded 1×10^5 ; for each eligible ion, the software enumerated molecular formulas within $\pm 2 \text{ ppm}$. Candidate compositions followed the notation $\text{C}_c\text{H}_h\text{O}_o\text{N}_n\text{S}_s$. Allowed atom counts were $\text{C} = 1\text{--}39$, $\text{H} = 1\text{--}72$, $\text{O} = 0\text{--}20$, $\text{N} = 0\text{--}7$, and $\text{S} = 0\text{--}4$. Additional chemical-plausibility filters limited *H/C* to 0.3–3, *O/C* to 0–3, *N/C* to 0–1.3, and *S/C* to 0–0.8 (Zhang et al., 2021).

2.4 H_2O_2 assay

H_2O_2 was quantified in aqueous filter extracts. A quarter of each filter was extracted for 15 min on a vortex shaker with

1.0 mL ultrapure water. Insoluble material was removed by centrifugation for 3 min at 9000 rpm (Eppendorf Minispin), and the supernatant was analyzed with a fluorometric kit from Sigma (Hydrogen Peroxide Assay Kit, MAK165). The assay protocol followed our earlier work (Tong et al., 2021, 2018). In each well of a 96-well plate, 50 μ L supernatant was combined with 50 μ L detection reagent containing Amplex Red substrate and horseradish peroxidase. Following a 30 min incubation, a Synergy™ NEO microplate reader (BioTek) recorded fluorescence at 540 nm excitation and 590 nm emission. Extract H_2O_2 concentrations were calculated from a calibration curve prepared with standard H_2O_2 solutions and corrected using blank measurements. Although the assay is designed for H_2O_2 quantification, potential contributions from other peroxide or oxygenated species in chemically complex aerosol extracts cannot be completely excluded.

2.5 EPR measurement of trapped radicals

Radical formation in the aqueous extracts of ambient PM and laboratory-generated SOA was quantified using EPR with a spin-trapping method, following the procedures established in our previous studies. For ambient PM samples, a section representing 25 % of the filter was used, while the complete SOA-loaded filter was processed for laboratory-generated SOA samples. Each filter was immersed in 10 mM BMPO (Enzo Life Sciences GmbH; high-purity 5-tert-butoxycarbonyl-5-methyl-1-pyrroline N-oxide), which acted as the radical trap, and agitated for 15 min on a Heidolph Reax 1 vortex shaker. During this process, short-lived radicals present in PM extracts were assumed to rapidly react with BMPO to form stable radical adducts suitable for EPR detection (Villamena and Zweier, 2002; Mitchell et al., 2013).

Adduct spectra were recorded for identification and quantification on an EMXplus-10/12 continuous-wave X-band instrument (Bruker Corporation). Consistent with earlier work, acquisition settings were a 100 G magnetic-field span; 100 kHz modulation at 1.0 G amplitude; 2.1 mW microwave power (20 dB); 40 dB receiver gain; and 50 accumulated scans. Radical concentrations were obtained through spectral fitting and spin counting in the Bruker Xenon software package.

2.6 Quality assurance and quality control

For UHRMS analysis, blank samples were analyzed to identify and remove background features, and molecular formulas were assigned using the mass-error and chemical-plausibility criteria described above. A mixture of standards of 12 organic compounds covering a wide range of molecular weights (122–230 Da) and polarity (retention time from 1.34 to 7.12 min) was regularly measured to confirm the stability of the analytical method. The mean variability of retention

time was less than 10 s, while the mean relative standard deviation of the peak intensity was less than 15 %.

For H_2O_2 measurements, concentrations were determined using calibration curves prepared with H_2O_2 standards, with blank measurements used for background correction. For EPR measurements, blank samples were analyzed under the same conditions as the aerosol extracts to account for background signals. All samples within each analysis were processed using the same analytical protocols and data-processing procedures to ensure consistency across sites and experiments.

3 Results and Discussion

3.1 MCR-VK-based molecular classification of OOC and UOC in ambient fine PM and laboratory-generated SOA

The UHRMS technique has become a powerful tool for characterizing the molecular composition of OA, enabling the assignment of elemental formulas to thousands of individual compounds in highly complex samples. To extract structural insights from UHRMS datasets, several metrics derived from elemental composition, such as DBE, aromaticity index (AI), and aromaticity equivalent (X_c), have been widely applied to capture unsaturation and aromaticity (Koch and Dittmar, 2006; Yassine et al., 2014; Steimer et al., 2020). We recently introduced MCR to estimate the maximum possible contribution of carbonyl-/epoxide-type functionalities based solely on molecular formula information (Zhang et al., 2021). For a given molecular formula of $\text{C}_c\text{H}_h\text{O}_o\text{N}_n\text{S}_s$, MCR is defined as the ratio of DBE to the number of oxygen atoms (O) when $\text{O} \geq \text{DBE}$, while MCR is set to unity when $\text{O} < \text{DBE}$. The equation of MCR is shown below:

$$\text{MCR} = \frac{\text{DBE}}{\text{O}}, \text{ for } \text{O} \geq \text{DBE} \quad (1)$$

$$\text{MCR} = 1, \text{ for } \text{O} < \text{DBE} \quad (2)$$

By integrating MCR into the traditional VK diagram, we developed the MCR-VK framework, which enables classification of OA compounds into chemically meaningful groups (Zhang et al., 2021). As shown in Fig. 1, the MCR-VK diagram is divided into two major areas by an MCR threshold of 0.9. Compounds with $\text{MCR} < 0.9$ are classified as OOC, while those with $\text{MCR} \geq 0.9$ are classified as UOC. The OOC comprise a wide range of oxygen-rich species, including very highly oxidized compounds such as organic peroxides and isoprene epoxydiols (IEPOX)-derived products, highly oxidized multifunctional molecules (e.g., 2-methyl-1,2,3-butanetricarboxylic acid (MBTCA) and other HOMs), and intermediately oxidized products such as pinic and pinonic acids derived from monoterpene oxidation (Fig. S2) (Yasmeen et al., 2012; Müller et al., 2012; Nguyen et al., 2014; Zhang et al., 2021; Mutzel et al., 2015). In contrast, UOC

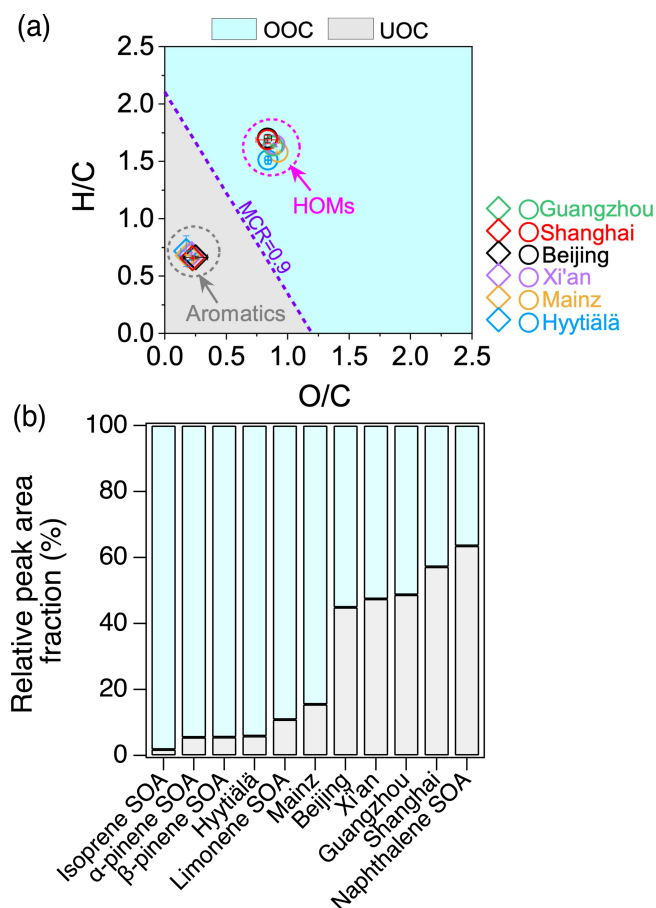


Figure 1. (a) MCR-VK diagram to classify organic compounds in atmospheric aerosols. The dashed line represents the boundary ($MCR = 0.9$) between the oxidized organic compounds (OOC, $MCR < 0.9$, cyan area) and unsaturated organic compounds (UOC, $MCR > 0.9$, grey area). Dots and diamonds indicate the positions of highly oxygenated molecules (HOMs) and aromatics identified in ambient fine PM samples. (b) Relative peak area-weighted fractions of OOC and UOC in ambient fine PM samples and laboratory-generated SOA.

are dominated by oxidized unsaturated compounds, including aromatic SOA products, combustion-related organics, and species formed through condensational aging processes (Fig. S2) (Zhang et al., 2021; Srivastava et al., 2022; Al-Naiema et al., 2020; Chan et al., 2009).

Figure 1b summarizes the relative peak-area-weighted fractions of OOC (RF_{OOC}) and UOC (RF_{UOC}) in ambient fine PM and laboratory-generated SOA samples, averaged for each site or experiment. Representative mass spectra and MCR-VK diagrams in ambient fine PM and laboratory-generated SOA samples are shown in Figs. S3 and S4, respectively. Note that because ESI response can vary among compounds, these peak area-weighted fractions should not be interpreted as quantitative measures of the actual abundance or mass fractions of OOC and UOC. Instead, they are

used here as relative molecular-composition metrics based on the detected compounds. The resulting relative fractions show distinct differences in OA composition across precursor types and environments (Fig. 1b). Isoprene SOA exhibits the highest RF_{OOC} (98 %), consistent with its dominant formation of highly oxygenated, low-MCR products such as 2-methyltetrols, in which most oxygen atoms are present as hydroxyl groups (Wang et al., 2018b; Surratt et al., 2010; Zhang et al., 2023; Surratt et al., 2006). Similarly, α -pinene and β -pinene SOA are overwhelmingly composed of OOC (95 % and 94 %, respectively), reflecting the prevalence of oxygen-rich ozonolysis products such as pinonic acid, pinic acid, nopinone, and MBTCA (Müller et al., 2012; Zhang et al., 2015; Mutzel et al., 2021; Fan et al., 2020). The fine PM samples collected in the boreal forest at Hyytiälä also exhibit a high RF_{OOC} (94 %), comparable to that observed in monoterpene-derived SOA, reflecting the dominant contribution of biogenic precursors, particularly α - and β -pinene, to SOA formation at this site (Kourtchev et al., 2013; Roldin et al., 2019; Kourtchev et al., 2014; Petäjä et al., 2022).

In contrast, naphthalene SOA is characterized by a substantially higher RF_{UOC} (64 %), indicating a strong contribution from aromatic, ring-retaining oxidation products. This observation is consistent with previous studies showing that naphthalene photooxidation under conditions of low nitrogen oxides (NO_x) predominantly yields aromatic quinones and ring-opening products while largely retaining at least one benzene ring (Kautzman et al., 2010; Lannuque and Sartelet, 2024). Urban fine PM samples display a wide range of RF_{UOC} (15 %–57 %), reflecting the diversity of emission sources and atmospheric processing pathways in urban environments. Samples from Chinese megacities of Beijing, Xi'an, Guangzhou, and Shanghai exhibit particularly high RF_{UOC} (45 %–57 %), indicating a substantial contribution from aromatic and combustion-related organics. This result agrees with our previous findings that mono- and polyaromatic compounds constitute a major fraction of OA in Chinese megacities (Wang et al., 2021). In contrast, fine PM samples from Mainz show substantially lower RF_{UOC} (15 %), suggesting a weaker contribution of aromatic emissions and a relatively greater biogenic influence compared with Chinese megacities, which is consistent with our previous study showing fewer compounds with high degree of unsaturation observed in Mainz OA compared to Beijing OA (Wang et al., 2018a).

To assess whether the MCR-VK-based classification reflects intrinsic molecular functionality, we further examined its relationships with complementary molecular indicators derived from the UHRMS data. Aromatic compounds and HOMs were identified from the assigned molecular formulas using established UHRMS-based criteria (Tong et al., 2019; Yassine et al., 2014). As shown in Fig. 1a, the aromatics of ambient fine PM samples from all sampling sites cluster within the UOC region in the MCR-VK diagram based on their average O/C and H/C values, whereas HOMs con-

sistently fall within the OOC region, reflecting their distinct degrees of unsaturation and oxygenation. Importantly, the MCR-VK-based classification shows strong quantitative agreements with these complementary molecular indicators. Across all samples, the RF_{OOC} correlates well with the relative fraction of HOMs ($R^2 = 0.75$, Fig. 2a), while the RF_{UOC} is strongly correlated with the relative fraction of aromatics ($R^2 = 0.88$, Fig. 2b). These strong correlations arise from clear environmental contrasts, whereby biogenic-influenced sites show high fractions of HOMs and low aromatic contributions, while urban megacities exhibit the reverse trend. Moreover, the ratio of OOC to UOC fractions (RF_{OOC} / RF_{UOC}) correlates well with the ratio of HOMs to aromatic fractions ($R^2 = 0.92$, Fig. 2c), further demonstrating that the framework captures the balance between unsaturated, aromatic moieties and oxygen-rich, multifunctional compounds. Collectively, these results indicate that the MCR-VK-based classification reflects underlying molecular functionality. Importantly, unlike HOM or aromatics identification, which requires specific compositional criteria and captures only a subset of organic compounds, the OOC/UOC classification encompasses the entire detected OA composition and therefore provides a more comprehensive representation of molecular functionality relevant to ROS formation.

3.2 ROS yields and formation potential of ambient fine PM and laboratory-generated SOA

Figure 3a compares the volume-normalized ROS yields (H_2O_2 + radicals) together with fine PM mass concentrations across all ambient sites. Substantial site-to-site variability is observed, reflecting differences in both aerosol loadings and atmospheric environments. Urban megacities such as Beijing, Guangzhou, Shanghai, and Xi'an exhibit substantially higher volume-normalized ROS yields (57.8 – $260.5 \text{ pmol m}^{-3}$) than the boreal forest site at Hyytiälä (13.0 pmol m^{-3}) and the semi-urban site in Mainz (49.9 pmol m^{-3}). This spatial pattern exhibits a similar trend with the corresponding fine PM mass concentrations (Fig. 3a), indicating that environments with higher particle loadings contain greater amounts of ROS-generating substances per unit air volume (Gali et al., 2020; Lakey et al., 2016). Across all sites, H_2O_2 dominates the ROS budget, accounting for approximately 78 %–97 % of total ROS. For example, H_2O_2 yields reach $253.7 \text{ pmol m}^{-3}$ in Beijing and $148.0 \text{ pmol m}^{-3}$ in Guangzhou, whereas radical yields remain comparatively low ($\leq 10.6 \text{ pmol m}^{-3}$). A similar dominance of H_2O_2 is observed at Hyytiälä and Mainz, despite their much lower ROS yields. We further examined the relationship between volume-normalized ROS and fine PM mass concentration. Strong positive correlations are observed between fine PM mass and volume-normalized total ROS, H_2O_2 , and radical yields (Fig. S5). These correlations indi-

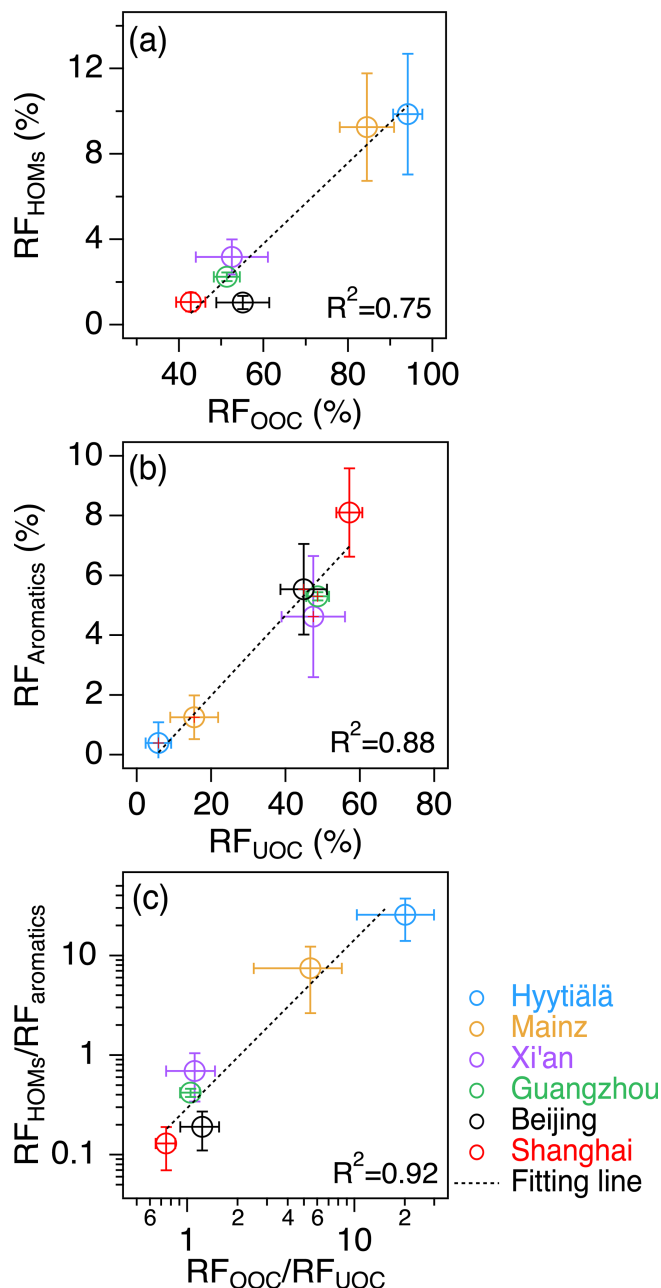


Figure 2. (a) Correlation between relative peak area-weighted fractions of OOC (RF_{OOC}) and HOMs (RF_{HOMs}); (b) correlation between relative peak area-weighted fractions of UOC (RF_{UOC}) and aromatics ($RF_{Aromatics}$); (c) correlation between the ratio of OOC to UOC fractions (RF_{OOC} / RF_{UOC}) and the ratio of HOMs to aromatic fractions ($RF_{HOMs} / RF_{Aromatics}$). The dots and error bars represent the mean values and standard deviations, respectively. The regression models, p values, and 95 % confidence intervals for the correlations are provided in Table S3.

cate that on an air-volume basis, ambient ROS exposure is largely governed by particle loading.

However, volume-normalized metrics alone do not capture intrinsic differences in the ROS formation potential of particles themselves. Figure 3b shows the mass-normalized ROS yields across all ambient sites, expressed as pmol of ROS per microgram of fine PM. The individual H_2O_2 , radical, and total ROS measurements underlying these site-averaged values are provided in Table S4. In contrast to the volume-normalized results, mass-normalized ROS yields show markedly different trends across sites and no longer scale with fine PM mass concentrations. For total ROS, the mass-normalized yields range from $0.73 \text{ pmol } \mu\text{g}^{-1}$ in Shanghai to $3.32 \text{ pmol } \mu\text{g}^{-1}$ in Mainz, with the boreal forest site at Hyytiälä also exhibiting relatively high values ($2.49 \text{ pmol } \mu\text{g}^{-1}$) despite its low fine PM mass concentration ($2.49 \text{ pmol } \mu\text{g}^{-1}$) despite its low fine PM mass concentration. This divergence clearly indicates that intrinsic particle composition, rather than particle mass, governs ROS formation on a per-mass basis. This observation further supports previous studies showing that intrinsic particle oxidative activity is more strongly governed by chemical composition than by PM mass concentration alone (Salana et al., 2024; Daellenbach et al., 2020). Across all sites, mass-normalized H_2O_2 yields dominate total ROS and exhibit a similar spatial pattern to total ROS, reflecting the widespread formation of relatively stable peroxide species in ambient fine PM. In contrast, radical yields exhibit a distinctly different behavior. Radical yields are the highest at the biogenic site Hyytiälä ($0.58 \text{ pmol } \mu\text{g}^{-1}$) and remain elevated in Mainz ($0.21 \text{ pmol } \mu\text{g}^{-1}$) but are substantially lower in some megacities such as Beijing ($0.07 \text{ pmol } \mu\text{g}^{-1}$) and Guangzhou ($0.11 \text{ pmol } \mu\text{g}^{-1}$). These differences point to pronounced variability in the chemical nature of fine PM across environments. The contrasting behaviors of H_2O_2 and radicals are further illustrated by their relative contributions to total ROS (Fig. S6). At Hyytiälä, radicals account for nearly one-quarter of total ROS (23 %), consistent with a greater contribution of reactive, short-lived ROS species in biogenic aerosols. In most urban environments, radical contributions are considerably smaller, typically around 7 %, and drop to as low as 3 % in Beijing. Notably, Shanghai exhibits a relatively high radical fraction (20 %) despite having the lowest total ROS yield, highlighting that radical contributions are not simply controlled by total ROS production but instead reflect distinct compositional features of the aerosol.

Correlation analysis further supports the interpretation that particle chemistry, rather than particle loading, governs intrinsic ROS formation potential. While volume-normalized ROS, H_2O_2 , and radical yields all show strong positive correlations with fine PM mass concentration, no significant correlations are observed between fine PM mass concentration and mass-normalized total ROS or H_2O_2 yields (Fig. S7a and b). In contrast, radical yields display a significant negative correlation with fine PM mass concentration ($R^2 = 0.90$, Fig. S7c). This inverse relationship indicates that although

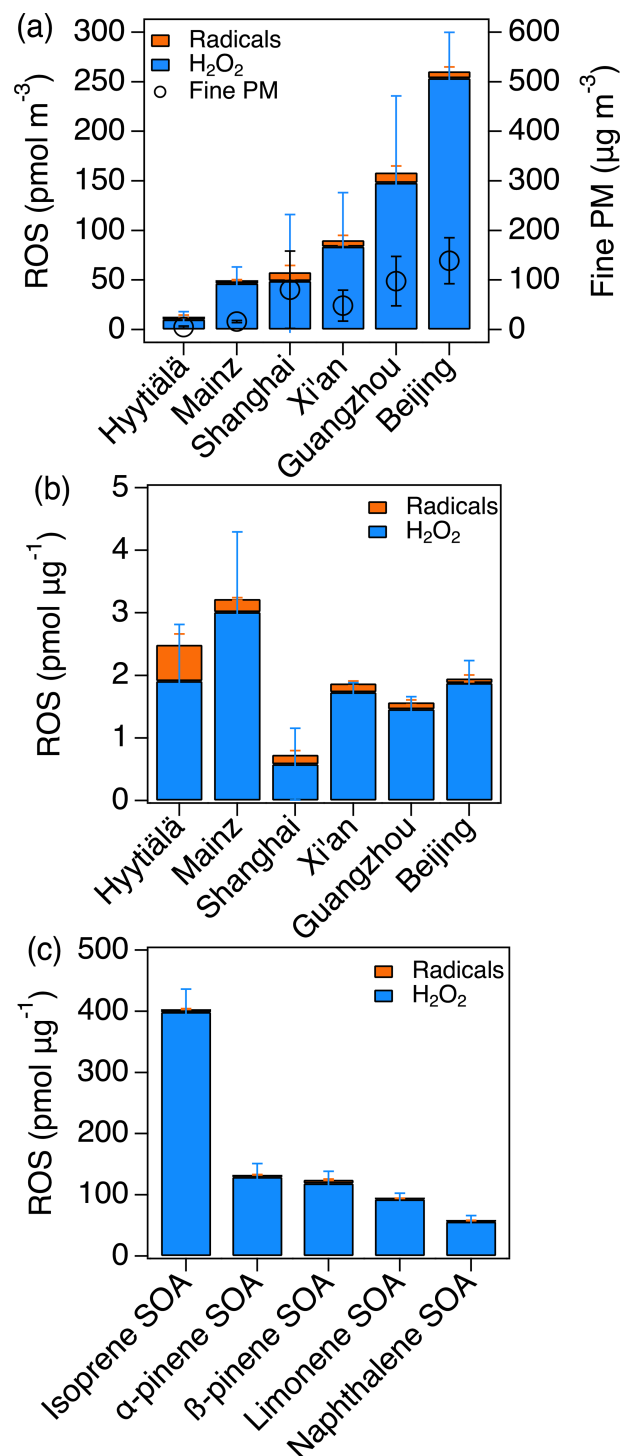


Figure 3. (a) The volume-normalized ROS yields (bars, H_2O_2 + radicals) and fine PM mass concentrations (dots) in ambient fine PM; (b) the mass-normalized ROS yields (H_2O_2 + radicals) in ambient fine PM; (c) the mass-normalized ROS yields (H_2O_2 + radicals) in laboratory-generated SOA. The error bars represent the standard deviations.

polluted environments generate higher total radical concentrations per unit air volume, individual particles in these environments are intrinsically less efficient at producing radicals. Conversely, particles in clean or biogenic environments, despite contributing less to the total atmospheric radical burden, exhibit a substantially higher radical yield on a per-mass basis. Interestingly, a similar negative relationship is observed between fine PM mass concentration and the $RF_{\text{OOC}}/RF_{\text{UOC}}$ derived from the MCR-VK classification ($R^2 = 0.87$, Fig. S7d). Urban megacities with high fine PM mass concentrations tend to exhibit lower $RF_{\text{OOC}}/RF_{\text{UOC}}$ values, consistent with a greater contribution from unsaturated, aromatic-rich organic aerosols. In contrast, biogenic-influenced sites characterized by lower fine PM mass show higher $RF_{\text{OOC}}/RF_{\text{UOC}}$ values, reflecting a dominance of highly oxygenated, multifunctional organic species (Huang et al., 2024; Roldin et al., 2019). The parallel trends observed for radical yields and $RF_{\text{OOC}}/RF_{\text{UOC}}$ suggest that environments favoring oxygen-rich OA composition also enhance the intrinsic capacity of particles to generate reactive radical species.

Laboratory-generated SOA provides additional context for interpreting these ambient patterns. Mass-normalized ROS yields of SOA derived from different precursors (Fig. 3c) span a wide range, with isoprene SOA exhibiting exceptionally high ROS yields ($403 \text{ pmol } \mu\text{g}^{-1}$), followed by α -pinene and β -pinene SOA ($125\text{--}133 \text{ pmol } \mu\text{g}^{-1}$), and substantially lower yields for limonene SOA ($94 \text{ pmol } \mu\text{g}^{-1}$) and naphthalene SOA ($58 \text{ pmol } \mu\text{g}^{-1}$). Although ROS yields of laboratory-generated SOA exceed those of ambient fine PM, the relative ordering among precursors provides a mechanistic framework for understanding ambient observations. Specifically, aerosols enriched in highly oxygenated, biogenic SOA components are expected to exhibit greater aqueous ROS-forming potential, whereas aerosols dominated by aromatic, less oxygenated organics are comparatively less efficient at generating ROS on a mass basis (Tong et al., 2018). This interpretation is consistent with the elevated mass-normalized ROS yields observed at Hyytiälä and the lower yields in megacities such as Shanghai and Beijing, despite the much higher aerosol mass loading in the latter. However, ROS-forming potential can depend on experimental conditions, including the extraction medium, pH, and assay endpoint. For example, Tong et al. (2018) reported medium-dependent ROS yields for naphthalene SOA in water and surrogate lung fluid, while Li et al. (2022) showed that pH strongly affected the peroxide content and oxidative potential of biomass-burning HULIS. Previous studies have also reported higher oxidative potential for anthropogenic aerosols, such as naphthalene SOA, than for biogenic SOA based on the dithiothreitol (DTT) assay (Tuet et al., 2017; Bates et al., 2019). This discrepancy likely arises because the DTT assay quantifies electron-transfer capacity and is sensitive to redox-active species such as quinones, whereas the present study measures hydrogen peroxide and radical formation in

aqueous extracts, reflecting product-based ROS formation pathways.

Overall, these results indicate that fine PM mass largely controls the total atmospheric ROS burden, whereas particle-level ROS formation potential is governed by OA composition. This contrast highlights the need for a molecularly resolved metric to link aqueous ROS-forming potential with OA chemistry.

3.3 Associations of $RF_{\text{OOC}}/RF_{\text{UOC}}$ with ROS yields in ambient fine PM and laboratory-generated SOA

To elucidate how molecular-level OA composition governs particle-level ROS formation, we examined the relationships between particle mass-normalized ROS yields (total ROS, H_2O_2 , and radicals) and the $RF_{\text{OOC}}/RF_{\text{UOC}}$ derived from the MCR-VK framework for both ambient fine PM and laboratory-generated SOA (Fig. 4).

For ambient urban fine PM samples (Mainz, Beijing, Xi'an, Guangzhou, and Shanghai), a strong positive exponential relationship ($R^2 = 0.94$, Fig. 4a) is observed between total ROS yields and $RF_{\text{OOC}}/RF_{\text{UOC}}$. Specifically, ROS yields increase rapidly with increasing $RF_{\text{OOC}}/RF_{\text{UOC}}$ at low to moderate values, followed by a gradual saturation at higher $RF_{\text{OOC}}/RF_{\text{UOC}}$. This behavior suggests that ROS formation may initially be limited by the availability of oxygenated organic functionalities and become progressively constrained by competing chemical pathways and interactions as oxidation increases. This saturation behavior may reflect the chemically complex nature of urban fine PM, in which diverse OA constituents, including unsaturated species, aromatics, and redox-active components, interact to regulate ROS generation efficiency. Further studies are needed to better understand the mechanisms underlying this nonlinear relationship. It should also be noted that OOC covers a chemically diverse range of compounds, which may differ in their ROS-forming activity. Because these yields are normalized to particle mass, the observed relationship directly reflects differences in chemical composition rather than particle loading. The consistency of this relationship across multiple cities with diverse emission profiles suggests that $RF_{\text{OOC}}/RF_{\text{UOC}}$ captures a fundamental compositional control on ROS generation that is robust across urban environments.

Given the dominance of H_2O_2 in the total ROS of ambient urban fine PM (80%–97%; Fig. S6), its dependence on OA composition closely follows that of total ROS. Accordingly, H_2O_2 yields exhibit a similarly strong positive relationship with $RF_{\text{OOC}}/RF_{\text{UOC}}$ ($R^2 = 0.98$, Fig. 4b), reinforcing that oxygenated organic enrichment strongly promotes aqueous ROS formation. Increases in OOC content therefore lead to higher mass-normalized ROS and H_2O_2 production. This behavior is consistent with previous studies showing that hydroperoxides, organic peroxides, and peroxy acids, functional groups commonly associated with OOC,

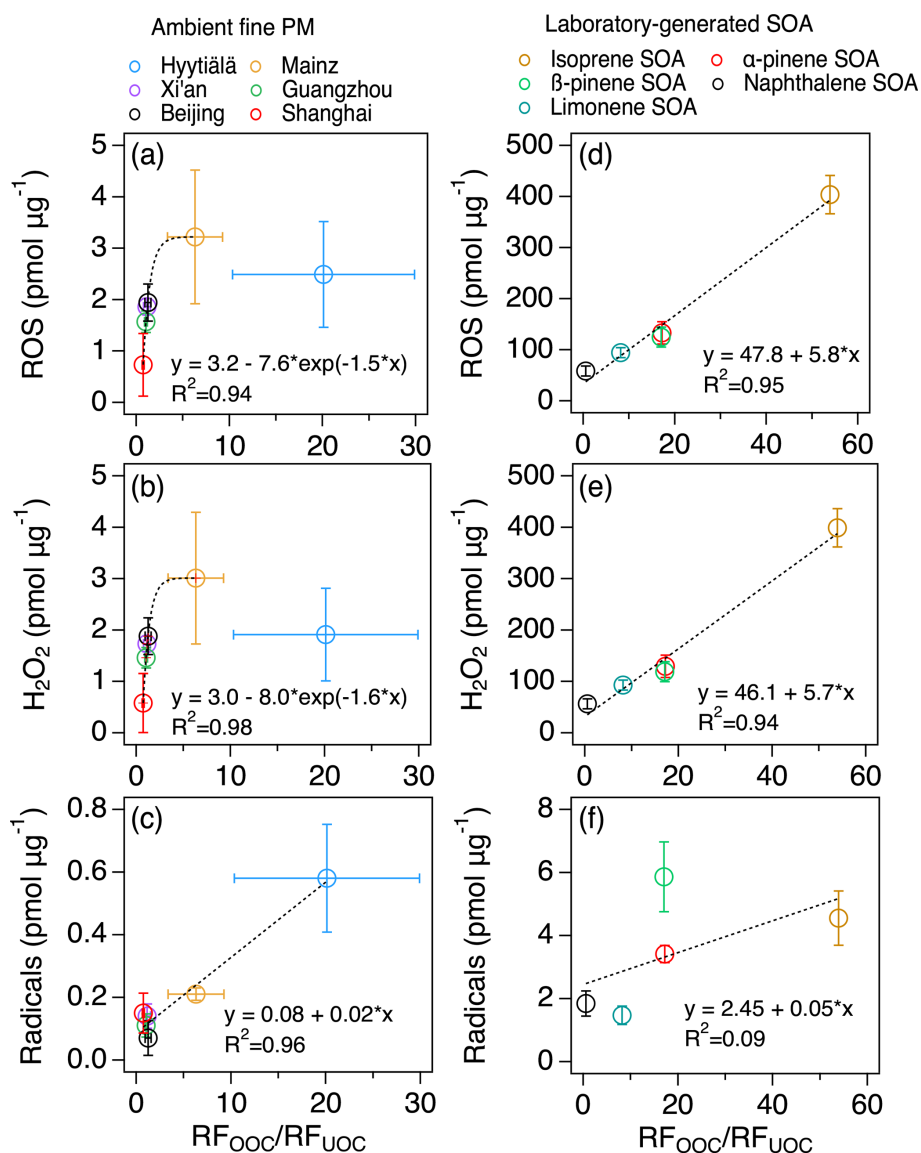


Figure 4. Correlations of mass-specific ROS yields (a, d), H₂O₂ yields (b, e), and radical yields (c, f) with RF_{OOC} / RF_{UOC} in ambient fine PM samples (a–c) and laboratory-generated SOA samples (d–f). The dots and error bars represent the mean values and standard deviations, respectively. The regression models, p values, and 95 % confidence intervals for the correlations are provided in Table S4.

can decompose or hydrolyze in aqueous environments to produce H₂O₂ (Wang et al., 2011; Tong et al., 2018; Hasson et al., 2001; Venkatachari and Hopke, 2008; Li et al., 2025). Liu et al. (2023) reported that the more oxidized oxygenated organic aerosols were associated with cellular ROS production, with highly unsaturated species containing carbon–oxygen double bonds and aromatic rings in OOA identified as important contributors. While oxidized organic species are found to play an important role in both studies, the present study links higher RF_{OOC} / RF_{UOC} to enhanced ROS formation. This difference likely reflects the different oxidative endpoints investigated. The previous study evaluated intracellular ROS responses, whereas the present study quantifies the intrinsic

formation of hydrogen peroxide and radicals in aqueous extracts.

An important deviation from the urban trend is observed for the boreal forest site at Hyytiälä. Although Hyytiälä fine PM exhibits a higher RF_{OOC} / RF_{UOC} ratio than urban samples, its H₂O₂ and total ROS yields fall below the exponential relationship established for urban aerosols (Fig. 4a and b). This behavior indicates that the empirical relationship derived for urban fine PM cannot be directly extrapolated to biogenic-dominated environments. The discrepancy likely reflects fundamental differences in aerosol composition and ROS-forming pathways. Urban fine PM typically contains higher abundances of quinones (classified as UOC),

which can substantially enhance H_2O_2 formation (Chung et al., 2006). In contrast, remote forest aerosols contain much lower abundances of metals and aromatic quinones, suggesting that ROS generation at Hyytiälä is dominated by biogenic SOA components.

Radical yields show a markedly different response to OA composition compared with H_2O_2 . For ambient fine PM, radical yields exhibit a positive linear relationship with $\text{RF}_{\text{OOC}}/\text{RF}_{\text{UOC}}$ when the biogenic site is included (Fig. 4c). This trend is largely driven by the elevated radical yields observed at Hyytiälä, where exceptionally high $\text{RF}_{\text{OOC}}/\text{RF}_{\text{UOC}}$ coincides with a high relative fraction of HOMs (Fig. 2). This behavior is consistent with our previous findings showing that HOMs, which are preferentially classified as OOC, can play an important role in aqueous radical formation (Tong et al., 2019). The enhanced radical yield at Hyytiälä likely reflects its HOM-rich OA composition. Among the urban sites, however, radical yields exhibit relatively limited variation despite differences in $\text{RF}_{\text{OOC}}/\text{RF}_{\text{UOC}}$, which could be due to additional influence by other aerosol constituents beyond the bulk balance between OOC and UOC. Therefore, $\text{RF}_{\text{OOC}}/\text{RF}_{\text{UOC}}$ may be more useful in predicting radical formation when comparing aerosols spanning contrasting source regimes (e.g., biogenic versus urban).

Laboratory-generated SOA further supports the compositional control inferred from the ambient observations. Across SOA formed from isoprene, α -pinene, β -pinene, limonene, and naphthalene, total ROS yields increase with the increase of $\text{RF}_{\text{OOC}}/\text{RF}_{\text{UOC}}$ and follow a strong positive linear relationship (Fig. 4d, $R^2 = 0.95$). A similar dependence is observed for H_2O_2 yields (Fig. 4e, $R^2 = 0.94$), consistent with the dominant contribution of H_2O_2 to total ROS in these systems. Unlike ambient urban PM, no saturation behavior is observed over the investigated compositional range, indicating that ROS formation in laboratory SOA remains composition-limited, with increasing oxygenation directly translating into greater aqueous ROS-forming potential under the present assay conditions. The absence of non-linear behavior further suggests minimal interference from competing redox-active components for SOA formed under control conditions.

In contrast, no clear relationship is found between radical yields and either $\text{RF}_{\text{OOC}}/\text{RF}_{\text{UOC}}$ for laboratory-generated SOA (Fig. 4f). This further suggests that radical formation depends more strongly on the abundance of specific radical-producing molecular species than on the overall balance between OOC and UOC. For example, semiquinone-type functionalities in naphthalene SOA can generate radicals through redox cycling pathways (Tong et al., 2019), leading to deviations from the overall composition–reactivity trends.

Since the $\text{MCR} = 0.9$ boundary was developed primarily for CHO compounds, we further performed a sensitivity analysis using only CHO formulas to assess whether the relationships described above were affected by its application to CHON, CHOS, and CHONS formulas (Fig. S8). For

the five ambient fine PM samples (Mainz, Beijing, Xi'an, Guangzhou, and Shanghai), the CHO-only $\text{RF}_{\text{OOC}}/\text{RF}_{\text{UOC}}$ ratio showed positive exponential relationships with total ROS ($R^2 = 0.87$; Fig. S8a) and H_2O_2 yields ($R^2 = 0.86$; Fig. S8b). When Hyytiälä was included, a positive linear relationship with radical yield was also observed ($R^2 = 0.96$; Fig. S8c). These relationships were consistent with those obtained using all molecular-formula classes ($R^2 = 0.94, 0.98$, and 0.96 , respectively), although the associations with total ROS and H_2O_2 were somewhat weaker. Thus, the observed composition–ROS relationships do not depend solely on the inclusion of heteroatom-containing formulas in the MCR classification. However, this sensitivity analysis does not independently validate the $\text{MCR} = 0.9$ boundary for CHON, CHOS, or CHONS compounds.

4 Conclusions and Implications

In this work, by applying the MCR-VK framework to a diverse range of ambient and laboratory aerosols, we show that the aqueous ROS-forming potential of fine PM is governed not by particle mass, but by the balance between two functionally distinct classes of organic compounds: OOC and UOC. The relative fraction of OOC compared with UOC is a key determinant of the ROS formation potential of fine PM. Particles enriched in OOC exhibit significantly higher mass-normalized ROS yields, particularly for H_2O_2 , indicating that the molecular composition of OA, rather than particle mass, governs aqueous ROS production.

As illustrated in Fig. 5, this compositional control leads to a clear contrast between urban and remote environments. In polluted urban areas, high PM mass concentrations result in elevated volume-normalized ROS, driving greater overall exposure to ROS. However, the aerosols themselves are less efficient at generating ROS per unit mass due to a relatively smaller contribution from OOC and a larger contribution from UOC. By contrast, in remote (e.g., forest) areas, lower particle loadings produce lower volumetric ROS, yet individual particles are intrinsically more reactive. This enhanced per-mass ROS formation is driven by the dominance of OOC (e.g., HOMs), leading to higher $\text{RF}_{\text{OOC}}/\text{RF}_{\text{UOC}}$ ratios. These results highlight that both particle mass and particle composition independently shape ROS formation, and both must be jointly considered when evaluating ROS-related health risks of ambient fine PM (Zheng et al., 2025; Salana et al., 2024).

The strong, consistent correlations between $\text{RF}_{\text{OOC}}/\text{RF}_{\text{UOC}}$ and mass-normalized ROS yields observed across urban megacities establish this ratio as a simple yet robust predictor for ROS formation potential of OA. Unlike previous studies that focused on specific ROS-active compound classes such as HOMs, organic peroxides, or quinones (Tong et al., 2019; Verma et al., 2015), the MCR-VK framework provides a generalized molecular-

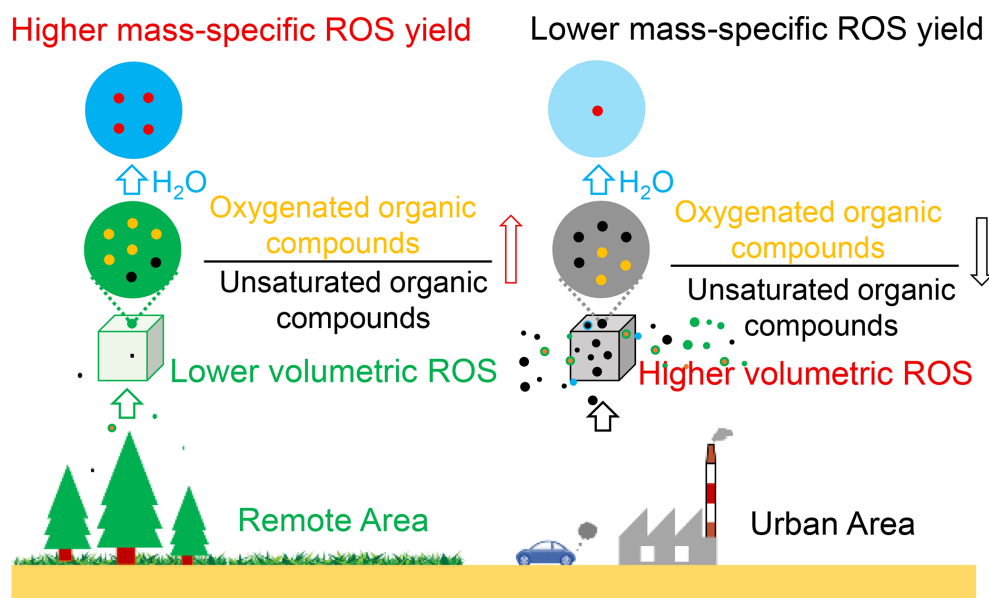


Figure 5. Schematic illustration of the relationships of volumetric ROS, the balance between oxidized and unsaturated organic compounds, and mass-normalized ROS yield of fine PM from remote and urban areas.

level descriptor that can be derived directly from UHRMS data without requiring targeted compound identification. This feature highlights the potential of the framework for application to chemically diverse atmospheric aerosols and offers a scalable approach for assessing aerosol oxidative activity. Within this framework, lower RF_{OOC}/RF_{UOC} corresponds to reduced mass-normalized ROS yields, while higher RF_{OOC}/RF_{UOC} likely indicates intrinsically more ROS-active aerosols. As a result, regional differences in precursor sources and atmospheric processing exert direct control over aerosol oxidative activity, providing a mechanistic explanation for the pronounced spatial variability in ROS formation. Laboratory-generated SOA provides further support for these conclusions. SOA formed from biogenic precursors such as isoprene and α -/ β -pinene, characterized by high RF_{OOC}/RF_{UOC} , exhibits the highest ROS formation efficiency, whereas SOA formed from naphthalene produces lower ROS yield per mass. Collectively, these ambient and laboratory results demonstrate that molecular composition, particularly the balance between OOC and UOC, provides a mechanistic basis for both the magnitude and spatial variability of ROS formation in atmospheric aerosols.

While this study focuses on the role of organic aerosol molecular composition, transition metals are also recognized contributors to ROS formation in ambient PM through metal-catalyzed redox cycling and Fenton-like reactions, particularly in urban environments (Charrier et al., 2014; Xiong et al., 2017; Tong et al., 2016). Interactions between redox-active metals and OA components, such as quinone- or peroxide-containing species, may further influence ROS formation pathways. However, the current analysis does not

quantitatively separate the contributions of OA and inorganic components to the measured ROS formation. In addition, ROS formation was quantified in aqueous extracts of particulate matter in this study, providing a chemically controlled system to evaluate ROS formation potential of aerosols and enabling consistent comparison across samples. However, simulated lung fluids may better represent physiological conditions due to antioxidants and metal-binding ligands, and future studies incorporating simulated lung fluids may refine the translation of ROS formation to more biologically relevant exposure metrics. Nevertheless, the strong and consistent correlations observed between ROS yields and RF_{OOC}/RF_{UOC} across diverse environments indicate that OA composition plays a critical role in particle-level ROS formation. Integrating molecularly resolved OA composition with metal speciation in future studies will be important for fully resolving their coupled and potentially synergistic effects (Charrier and Anastasio, 2015; Lin and Yu, 2026).

Overall, the MCR-VK framework offers a predictive, molecular-level approach to link OA composition with ROS formation potential. Future efforts should prioritize long-term, molecularly resolved measurements of OA across diverse environments, coupled with ROS assays, as well as concurrent, comprehensive, and complementary aerosol and aerosol precursor characterization during the sample collection, to capture the combined influence of particle loading, chemical composition, and atmospheric processing. Such integrated approaches will improve identification of the OA components most responsible for oxidative stress, advance understanding of the health risks associated with ambient

fine PM, and support the development of more targeted and composition-aware air quality management strategies.

Data availability. The data sets generated in the current study are available at Zenodo data repository at <https://doi.org/10.5281/zenodo.19334829> (Wang, 2026).

Supplement. Table showing the detailed information for the ambient particle sampling; figures showing the schematic outline of the experimental approach, maximum carbonyl ratio (MCR)-Van Krevelen (VK) diagram, detailed mass spectra and MCR-VK diagram for both ambient and laboratory-generated SOA samples, correlations of volume-normalized/mass-normalized ROS yield, H_2O_2 yield and radical yield with fine PM mass concentration, contributions of H_2O_2 and radicals to total ROS yield. The supplement related to this article is available online at <https://doi.org/10.5194/acp-26-14655-2026-supplement>.

Author contributions. This study was conceived by TH, KW and HT. YZ and KW conducted the sample analysis. SY, HK, TP, MK and PF assisted with the sample and data collections. FL and YZ wrote the original manuscript. All authors contributed to the final interpretation and writing of the manuscript.

Competing interests. At least one of the (co-)authors is a member of the editorial board of *Atmospheric Chemistry and Physics*. The peer-review process was guided by an independent editor, and the authors also have no other competing interests to declare.

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Acknowledgements. We thank Steven Lelieveld and Alexander Filippi for technical support.

Financial support. This work is supported by the National Natural Science Foundation of China (42475111), Natural Science Basic Research Program of Shaanxi Province (2026TS4JC-YXQN-099), Research Council of Finland flagship Atmosphere and Climate Competence Center (359340) and INAR RI (358647, 367739), the Helmholtz-Zentrum Hereon, and the Deutsche Forschungsgemeinschaft (ZH 511/8-1, HO 1748/23-1, HO 1748/19-1).

Review statement. This paper was edited by Quanfu He and reviewed by two anonymous referees.

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