

## **Responses to review comments-1 (RC1, by the Anonymous Referee #2)**

Review of Zhang et al. entitled “Particulate organic nitrates in eastern china: variation characteristics and effects of anthropogenic activities”

This study presents the measurements of six different organic nitrates in the particle phase in places in China that are representative of both urban and rural environments. The levels and diurnal patterns of these nitrates are reported and their correlations with other factors such as meteorological conditions and anthropogenic tracers are discussed. Overall, the paper is clearly written and reports the measurements of a very important SOA constituent in China. However, one is left with an impression that the manuscript is simply reporting values and numbers other than a thorough analysis of the sources and transformations of these organic nitrates in the atmosphere. Prior to publication the authors should endeavor to provide a more mechanistic and quantitative discussion about various physical and chemical conditions/factors associated with the observed patterns of organic nitrates at different sampling sites.

**Response:** we thank the reviewer for the critical comments and helpful suggestions. More discussion on physical and chemical mechanisms has been added in the revised manuscript to help to understand the observed variation patterns of monoterpene and oleic acid-derived particulate organic nitrates and the dominant influencing factors, including exploring the reasons for the diurnal difference, evaluating the impact of air mass transport, and supplementing additional evidences to the influencing factors. All of comments are responded in details as below.

General:

The manuscript has been largely improved in terms of the identification of organic nitrates using tandem mass spectrometry techniques. The observations of neutral losses of NO<sub>2</sub> and HNO<sub>3</sub> upon fragmentation of the parent ions certainly provide strong evidence for the presence of the -ONO<sub>2</sub> functional group in the analytes of interest. The quantification of organic nitrates, however, is a big limiting factor in the accuracy and reliability of the data presented here. While I understand that the authentic standards for most nitrates studied here are not available (not all of them though, some monoterpene derived nitrates can be synthesized), using surrogates as an alternative could certainly bring large uncertainties to the measurements, which need to be assessed carefully. Specifically, one important question to answer is that is the electrospray ionization efficiency of the surrogates (depends on which functional group is ionized) on the same order of magnitude as the compound of interest?

**Response:** thanks for the comments. It is rather difficult to determine the electrospray ionization efficiency of the surrogates, because the detachment cross section cannot be directly measured through the ESI/MS and the computing methods with regression models reported in some literatures are not

appropriate for multifunctional organic compounds. Therefore, we further test the response variations of the surrogate standards and ambient PONs in the mass spectrometer at different voltages to estimate the relative electrospray ionization efficiency. The ion source voltage is adjusted to 3000 V, 3500 V, 4000 V, and 4500 V. The results show that the variation in the mass spectrum response for surrogate standards and ambient PONs is relatively small when the voltage changes. Specifically, the average relative changes in the peak areas of the surrogate standard of (1R, 2R, 5R)-(+)-2-hydroxy-3-pinanone and monoterpene-derived organic nitrates are  $11.2\% \pm 3.0\%$  and  $11.4\% \pm 1.7\%$ , respectively. The average relative changes in the peak areas of the surrogate standard of ricinoleic acid and oleic acid-derived nitrates are  $9.3\% \pm 3.5\%$  and  $12.4\% \pm 1.7\%$ , respectively. The average relative changes in the peak areas of the surrogate standard of (-)-10-camphor sulfonic acid and pinene sulfate organic nitrate are  $8.8\% \pm 7.8\%$  and  $8.5\% \pm 7.0\%$ , respectively.

In addition, the responses of n-pentane, amyl nitrate, isosorbide, and isosorbide 5-nitrate in the mass spectrometer are measured to estimate the differences in the response caused by the nitrate functional group. The difference in responses of n-pentane and amyl nitrate is  $60.9\% \pm 7.2\%$ , and the difference between isosorbide and isosorbide 5-nitrate is  $66.6\% \pm 2.7\%$ . Indeed, there is an inherent difference in responses of surrogate standards and analytes. However, the nitrate group does not cause a difference more than one order of magnitude. In this study, the structures and the retention time of the surrogate standards we selected are very close to those of analytes. Therefore, in our view the electrospray ionization efficiencies of surrogates and analytes are generally similar, and the concentrations of organic nitrates can be estimated reasonably and further used for exploring the variation characteristics.

Line 186-191, *“The difference in the mass spectrum response caused by the nitrate functional group was estimated with n-pentane, amyl nitrate, isosorbide, and isosorbide 5-nitrate. The difference between n-pentane and amyl nitrate was  $60.9\% \pm 7.2\%$ , and the difference between isosorbide and isosorbide 5-nitrate was  $66.6\% \pm 2.7\%$ . Indeed, there is an inherent difference in responses of surrogate standards and analytes, and the nitrate group does not cause a difference more than one order of magnitude. Therefore, the concentrations of organic nitrates can be estimated reasonably and further used for exploring the variation characteristics.”*

The authors have spent almost the entire text describing the measurements of individual organic nitrates at different sampling sites: their concentrations during the day and nighttime, mass fractions in the total organic matters, and their correlations with other trace species like SO<sub>2</sub>. However, a mechanistic and quantitative exploration of the temporal variations and spatial distributions of different nitrates is lacking. A couple of examples:

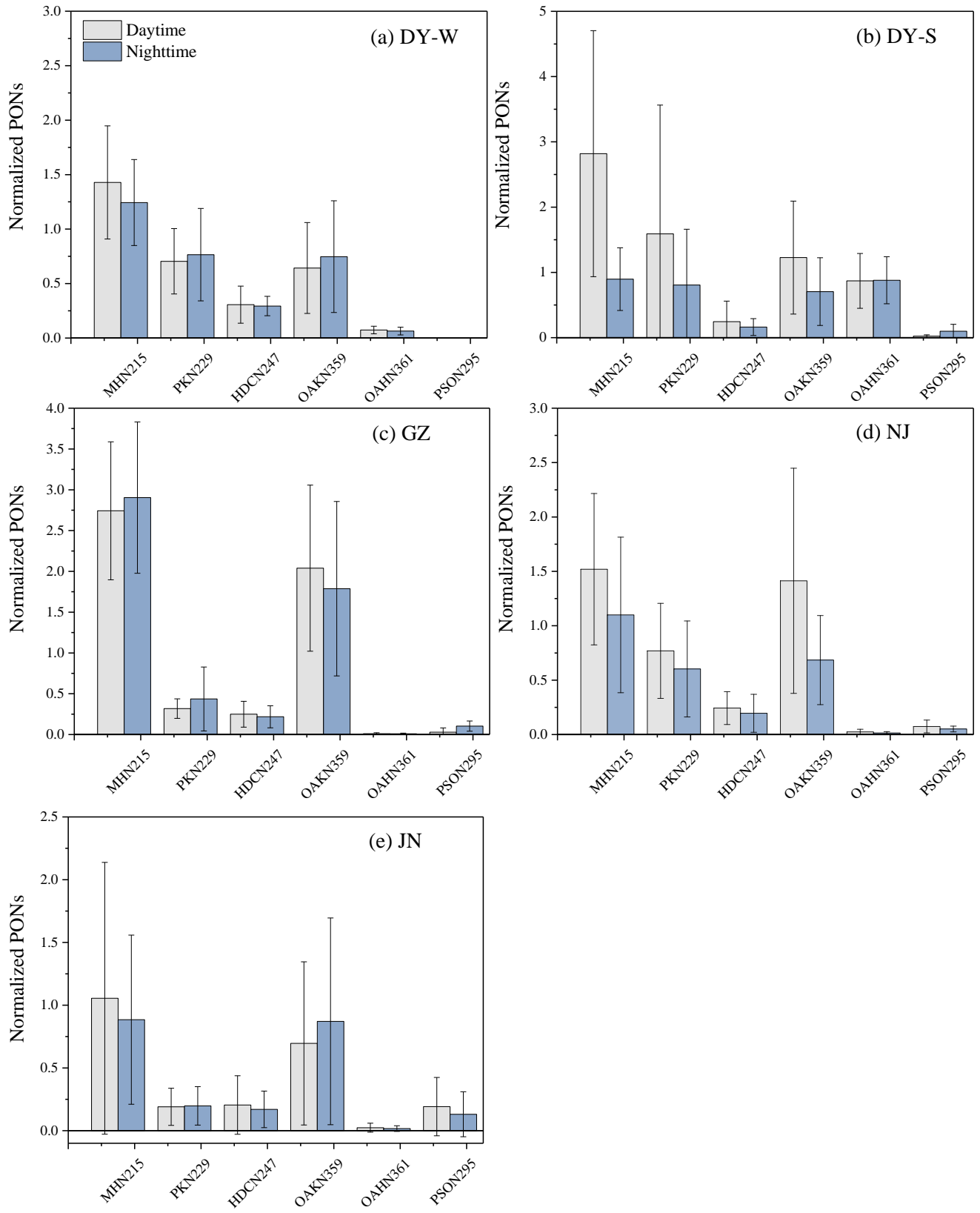
1. The entire section of 3.2 ‘Diurnal difference of PONs’ centers on discussing the different concentrations and patterns of organic nitrates in the day vs. night at different sampling sites. However, the mechanisms leading to such a pattern are barely explored. Figure 3 shows that the nighttime concentrations of MHN215 and PKN229 are only half of their daytime concentrations, in contrast to

almost all the other cases where the daytime and nighttime nitrate concentrations are quite comparable. It is well known that organic nitrates can be produced from NO<sub>3</sub>-initiated dark chemistry. A simple correlation analysis performed here does not provide any quantitative insights into the role of nighttime chemistry in the observed diurnal pattern of nitrates. The authors are suggested to do some calculations based on the NO<sub>x</sub> and O<sub>3</sub> measurements to assess the intensities of nighttime chemistry (including both ozonolysis and NO<sub>3</sub> oxidation) at different observational sites. Such a calculation is the first step to evaluate the contribution of nighttime chemistry to the production of organic nitrates.

**Response:** the possible mechanisms leading to diurnal difference and the calculation results have been added in the revised manuscript.

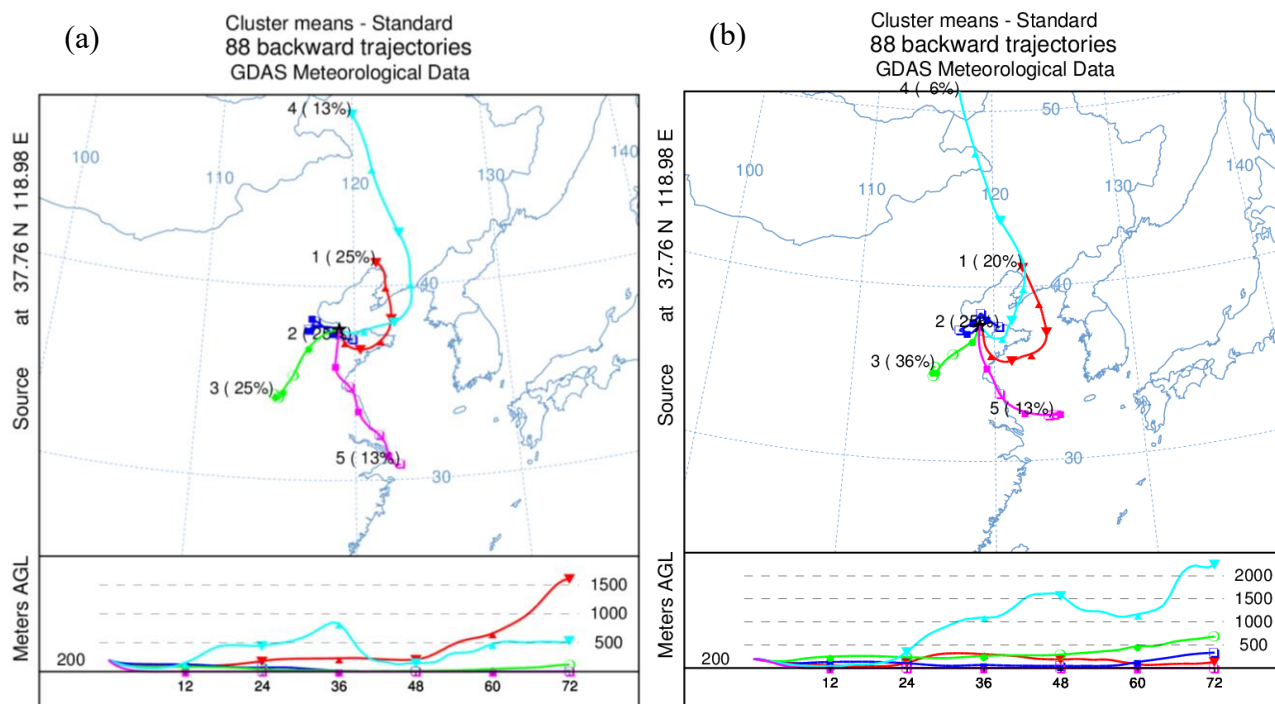
*Line 259–271, “Particularly, at the DY site in summer, MHN215 and PKN229 exhibited obviously higher contributions at daytime than those at nighttime ( $p < 0.01$ ). To verify whether the diurnal difference was aroused by the change in boundary layer height, the PONs/PM<sub>2.5</sub> ratios were also compared (see Fig. S3). The very similar diurnal trends between PON concentrations and PONs/PM<sub>2.5</sub> ratios suggest that the boundary layer change had little influence on the diurnal difference in the concentrations of PONs. Further cluster analysis (shown in Fig. S4) indicates that the air masses exhibited no significant difference between the daytime and nighttime sampling periods. It means that the diurnal difference was not mainly caused by air mass transport. Note that during daytime in summer at the DY site, biomass burning was intensive which can significantly increase the ozone concentration and enhance the atmospheric oxidation capacity (detailed discussion can be seen in Section 3.3.2). In addition, the emission rates of precursor monoterpenes were high at daytime due to the high temperature and the intense sunlight (Rinne et al., 2002). Therefore, the relative abundant oxidants and monoterpenes at daytime were ready to react to produce more monoterpenes-derived nitrates. For other kinds of organic nitrates, the concentrations during daytime and nighttime were comparable, that is consistent with the findings by Sobanski et al.(2017).”*

*Line 281–287, “To understand the role of nighttime chemistry playing in the abundances of organic nitrates, the nighttime production rate of organic nitrates was calculated via  $P_{\text{night}} = \alpha(\text{NO}_3)k_{(\text{NO}_2+\text{O}_3)}[\text{NO}_2][\text{O}_3]$  (Sobanski et al., 2017), in which  $\alpha(\text{NO}_3)$  is the yield of organic nitrates with NO<sub>3</sub>,  $k_{(\text{NO}_2+\text{O}_3)}$  is the rate coefficient for the reaction between NO<sub>2</sub> and O<sub>3</sub> and is determined by  $1.4 \times 10^{-13} \exp(-2470/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ . The  $\alpha(\text{NO}_3)$  reported in previous studies varies with precursors from 0.22 to 0.54 (Hallquist et al., 1999; Fry et al., 2009; Fry et al., 2011; Fry et al., 2014), and the mean value of 0.4 is adopted here. Based on the above calculations, the average nighttime production rates of PONs at the JN site and the DY site in summer were  $381 \pm 400 \text{ ppt h}^{-1}$  and  $362 \pm 157 \text{ ppt h}^{-1}$ , respectively, which are fast enough to produce the observed PON concentrations.”*



**Figure S3.** The differences in PONs/PM<sub>2.5</sub> ratios during daytime and nighttime at different sampling

sites.



**Figure S4.** Air mass clusters classified by the 72-h backward trajectories at (a) daytime and (b) nighttime at the DY site in summer during the sampling period.

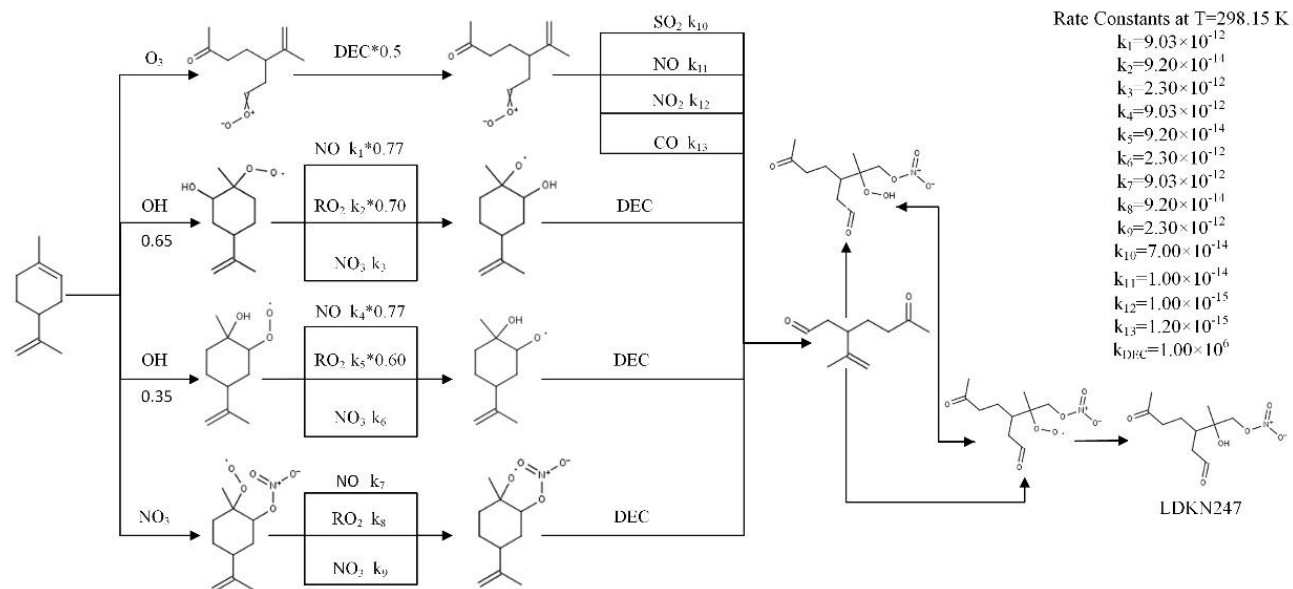
2. The authors observed a positive correlation between organic nitrates and SO<sub>2</sub> and attributed such a correlation to that reactions of SO<sub>2</sub> with stabilized Criegee intermediates produced from ozonolysis of monoterpenes could potentially promote the formation of organic nitrates. Such a conclusion is rather hasty and needs further observational evidence as support. The authors need to first consider: Are there any positive correlations between organic nitrates and other anthropogenic tracers such as NO<sub>x</sub> and CO? Are the temporal variations of organic nitrates simply a result of a sequence of pollution episodes caused by for example, high emissions or stagnant meteorological conditions? Furthermore, it is very important to keep in mind that the products from SCI+SO<sub>2</sub> reactions are not necessarily low in vapor pressure and thus constituting potential precursors of SOA, not to mention that the stable products from SCI+SO<sub>2</sub> reactions do not contain any -ONO<sub>2</sub> functional groups and further oxidation steps are required to produce organic nitrates. Such a hypothetical reaction scheme is inconsistent with the chemical structures proposed for each nitrate listed in Table 1, which suggest that most organic nitrates identified, at least those monoterpene derived nitrates, are first generation products from OH/NO<sub>3</sub> initiated oxidation of monoterpenes.

**Response:** at the DY site in winter, PONs was moderately correlated with CO ( $r = 0.61$ ,  $p < 0.01$ ). At the JN site the correlation between PONs and NO<sub>2</sub> or CO was negligible or weak ( $r = 0.17$ ,  $p < 0.41$  and  $r = 0.43$ ,  $p < 0.05$ , respectively). On the basis of the observation data, the effect of air mass transport cannot be entirely ruled out. However, when compared with the strong correlation between SO<sub>2</sub> and

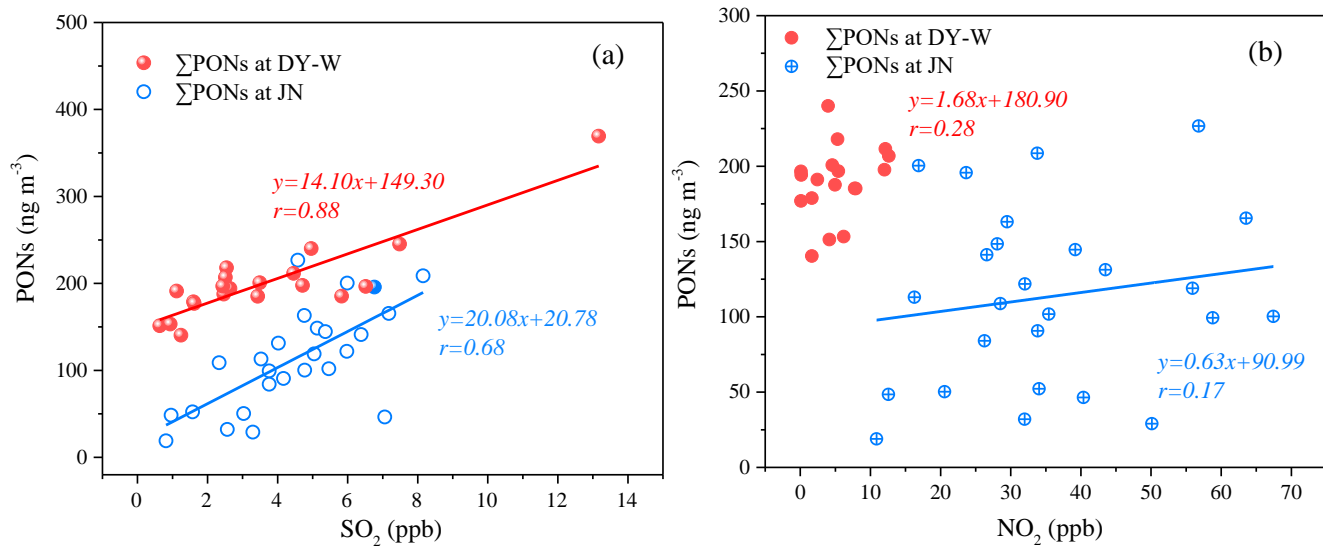
organic nitrates at the JN site and the DY site in winter ( $r=0.68$  and  $0.88$ , respectively;  $p<0.01$ ), air mass transport is assumed to have no controlling effect on the variation of organic nitrates, especially at the JN site. Here, we further examine the correlation between the concentrations of  $\text{SO}_2$  and PONs at the JN site after deducting the effect of transport. According to the linear fitting of the data of PONs and CO, the part of PONs which was associated with air mass transport is estimated by  $[\text{PONs}]_{\text{trans}}=69.27 \times [\text{CO}] + 55.38$ . Based on the observed concentrations of PONs and CO, the concentration of locally produced PONs is roughly calculated by subtracting the portion from air mass transport. The moderately strong correlations between estimated locally formed PONs and  $\text{SO}_2$  ( $r=0.64$ ;  $p < 0.01$ ) confirm the large effect of coal combustion on the formation of PONs. In addition, the average concentrations of  $\text{PM}_{2.5}$  at the JN site in autumn and at the DY site in winter were  $69.5 \pm 42.5 \text{ ng/m}^3$  and  $77.8 \pm 51.8 \text{ ng/m}^3$ , respectively, with the ranges of  $10.0\text{--}151.1 \text{ ng m}^{-3}$  and  $37.8\text{--}229.4 \text{ ng m}^{-3}$ , respectively. As indicated by the temporal variations of  $\text{PM}_{2.5}$  in Figure 5, there were no continuous and severe pollution episodes during the sampling periods.

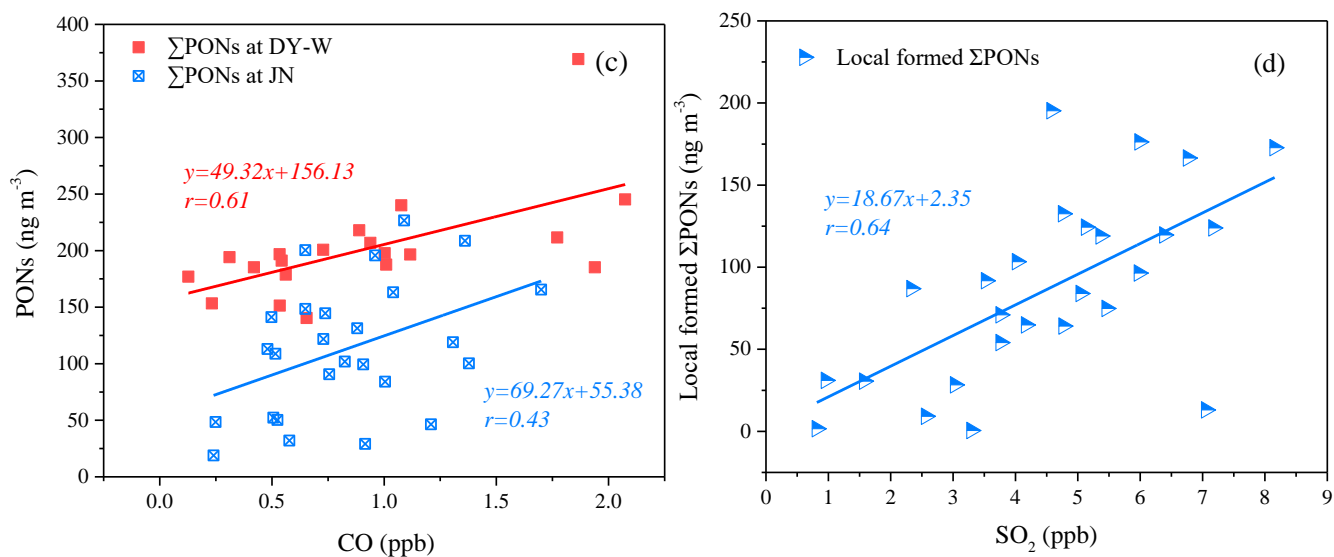
The reaction scheme of limonene with ozone, OH, and  $\text{NO}_3$  to produce LDKN247 (i.e. HDCN247 in the revised manuscript) in the gas phase (shown in Fig. S7) is adopted from the Master Chemical Mechanism version 3.3.1 (MCM, <http://mcm.leeds.ac.uk/MCM/>). The gas-phase ozonolysis of limonene firstly generates CIs. The CI then reacts with  $\text{SO}_2$  (or NO,  $\text{NO}_2$ , or CO) to form 3-isopropenyl-6-oxoheptanal, and finally produces LDKN247. The produced gas-phase LDKN247 is ready to partition into the particle phase. According to the predicted vapor pressure of 0.06 mmHg at 25 °C (predicted from the website of ChemSpider, available at <http://www.chemspider.com/Chemical-Structure.2282909.html?rid=6fa367c1-85d1-4d19-83c2-e5fb2fb5466a>), the product of 3-isopropenyl-6-oxoheptanal from SCI and  $\text{SO}_2$  is semi-volatile and readily further reacts with  $\text{NO}_3$  and OH at the rate constants of  $2.6 \times 10^{-13}$  and  $1.1 \times 10^{-10}$  at 298K, respectively. Therefore, the formation pathway of particulate organic nitrates from the reactions of CIs with  $\text{SO}_2$  is feasible.

Line 334–342, “At the DY site in winter, PONs was moderately correlated with CO ( $r = 0.61$ ,  $p < 0.01$ , see Fig. 6 (c)), which indicates that the transport possibly had an effect on the concentration of PONs. However, the relationship between PONs and  $\text{NO}_2$  or CO was negligible or weak ( $r = 0.17$ ,  $p < 0.41$  and  $r = 0.43$ ,  $p < 0.05$ , respectively) at the JN site. It means that transport was not the controlling factor for the strong correlation between PONs and  $\text{SO}_2$ . With an assumption that the PONs were partly affected by transport and this portion was linked to the CO concentration, the PONs associated with air mass transport was roughly estimated by  $[\text{PONs}]_{\text{trans}}=69.27 \times [\text{CO}] + 55.38$ . The locally produced PONs was then approximated by subtracting the part from transport. As shown in Fig. 6 (d), the moderately strong correlation between locally formed PONs and  $\text{SO}_2$  confirms the large effect of coal combustion on the formation of PONs during the measurement periods.”



**Figure S7.** Formation mechanisms of HDCN247 from limonene adopted from the Master Chemical Mechanism (MCM).





**Figure 6.** Scatter plots and the correlations between PONs and (a) SO<sub>2</sub>, (b) NO<sub>2</sub>, and (c) CO and between (d) locally generated PONs and SO<sub>2</sub> at the DY site in winter and at the JN site.

Specific:

Page 1, Line 25-30: Please carefully evaluate whether or not the SCI+SO<sub>2</sub> reactions are associated with the observed nitrate production in the particle phase.

**Response:** some additional discussion on the impact of SO<sub>2</sub> on PONs formation has been added in the revised manuscript (Section 3.3.1), and the related description has been clarified as follows.

Line 28–30, “Industrial and residential coal combustion played an important role in the increased concentrations of PONs through providing the related reactants and interfaces and promoting the formation rates of PONs.”

Page 2, Line 42: Clarify here oleic acid is mostly of anthropogenic origin.

**Response:** oleic acid has been deleted from this sentence.

Line 41–45, “*The biogenic volatile organic compounds (BVOCs) isoprene, monoterpenes, and sesquiterpene have been identified as major precursors of PONs and the production yields are dramatically different with BVOC species (Fry et al., 2014; Boyd et al., 2015). Oleic acid, one of the most common fatty acid found in animals and plants, is recognized as a tracer for anthropogenic cooking aerosols and is also considered to be a precursor of organic nitrates (Docherty and Ziemann, 2006).*”

Page 2, Line 49: Compounds with low vapor pressure are more likely condensing to particle phase and thus recognized as potential SOA precursor.

**Response:** yes, it has been modified.



Line 49–50, “*Once formed, highly functionalized nitrates are expected to partition to the particle phase due to their low vapor pressure (Lim and Ziemann, 2005).*”

Page 2, Line 51: The references cited here are for the organic sulfate formation under acidic conditions, not nitrates.

**Response:** one of the compounds studied in Surratt et al. (2008) is nitrooxy organosulfate, i.e., pinene sulfate organic nitrate (PERSON295) in our study, so we cited it here. Another reference of Han et al. (2016) indicated that particle acidity facilitated the formation of particulate organic nitrates. In the revised manuscript, the former reference has been removed and the latter reference is retained.

Line 51–52, “*Moreover, laboratory studies have shown that organic nitrates can be formed heterogeneously by acid-catalyzed reactions (Han et al., 2016).*”

Page 4, Line 139: Methanol is considered a very polar solvent, similar to water. Have the authors found any evidence of nitrate hydrolysis in pure methanol solvent? Have the authors tried to use some nonpolar solvents such as acetonitrile? Any difference in terms of the quantification of organic nitrates?

**Response:** the hydrolysis rate constant of organic nitrates will increase with solution acidity. During the hydrolysis of the  $\alpha$ -pinene-derived nitrate, a proton is abstracted by water molecule and then final products are produced (Rindelaub et al., 2016). However, because of the electron donating effect of methyl, the H in the hydroxyl group of methanol is not as active as the H in water. Therefore, methanol is commonly used as the extraction solvent and eluent for organic compounds. In this study, no apparent hydrolysis was observed by using pure methanol solvent. Actually, we have used acetonitrile as potential solvent when we try to establish the analytical method; however, there is no significant difference in the extracting efficiency and the mass spectrum response between acetonitrile and methanol. In fact, the polarity of acetonitrile and methanol are very close. With consideration of the strong elution capacity for hydroxyl-containing substances and the low toxicity, methanol is eventually selected as the solvent to extract the organic nitrates in ambient particulate samples.

Line 138–139, “*Methanol and acetonitrile have similar polarities. Due to the low toxicity and good solubility for hydroxyl-containing compounds, methanol was eventually selected as the extraction solvent.*”

Page 5, Line 160-165: Please explain why some nitrates have neutral losses of NO<sub>2</sub> while others have HNO<sub>3</sub> losses upon fragmentation?

**Response:** the different fragments are associated with the analytes’ structures. The C-O bond is easier to break than the O-N bond, especially after adding the hydrogen to the hydroxyl group at  $\beta$ -carbon (see Fig. R1). As a result, it is common to see fragments of NO<sub>3</sub> and HNO<sub>3</sub> when the analyte contains nitrate groups. However, monoterpene-derived organic nitrates have denser electron clouds due to the ring structure, so the C-O bond is more stable than the O-N bond. For this reason, the O-N bond is ready to

break and produce the fragment of  $\text{NO}_2$ . The difference in fragments in this study is consistent with the mass spectrum analysis of oleic acid-derived organic nitrates and monoterpene-derived organic nitrates in previous studies by Docherty and Ziemann (2006) and Perraud et al. (2010), in which  $\text{HNO}_3$  loss was found in the MS/MS spectra of oleic acid-derived organic nitrates and  $\text{NO}_2$  losses was observed in the MS/MS spectra of the pinene-derived organic nitrate.

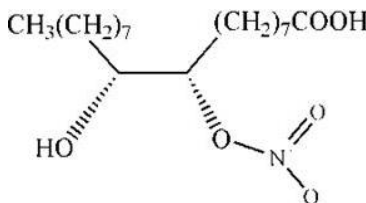
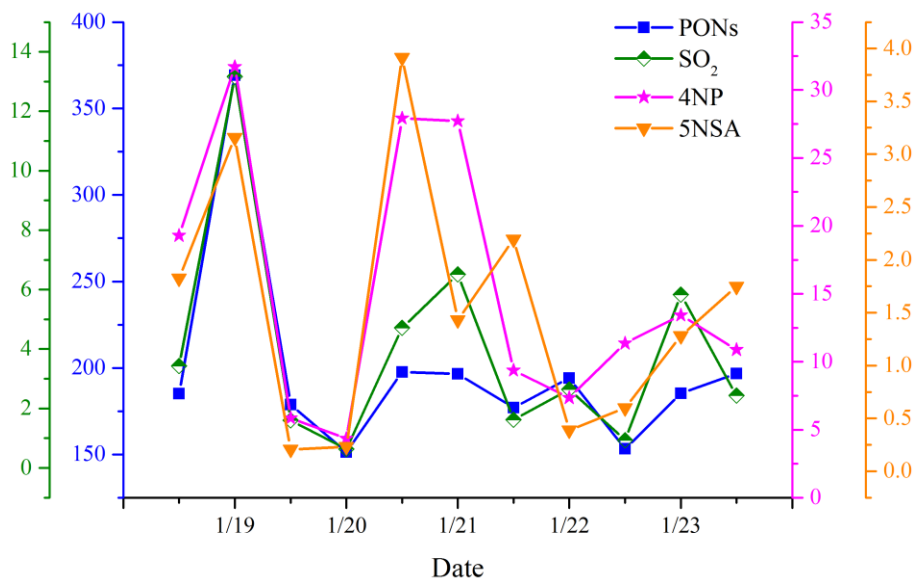


Figure R1. The molecular structure of the oleic acid hydroxyl nitrate

Page 7, Line 280-285: Unless the measured nitrates are representative of unique tracers of coal burning aerosols, or other identified tracers of coal burning exhibited strong correlations with the nitrates, it is otherwise an invalid conclusion that the increase of PONs is due to coal burning activities.

**Response:**  $\text{SO}_2$  was used as a good tracer for coal combustion plumes. With examination of the backward trajectories (see Fig. S5) and the locations of coal combustion industries, it can be deduced that the elevated levels of  $\text{SO}_2$  came from coal combustion emissions in urban and suburban Jinan. The strong correlation between  $\text{SO}_2$  and PONs (see Fig. 6) indicates the elevated concentration of PONs was to some content associated with the coal combustion activities. At the DY site in winter, there are rare coal combustion industries near the sampling site. We suppose that the  $\text{SO}_2$  was from the residential coal burning for heating demand. Here, several nitrated phenols which are abundant in coal combustion flue gas (Lu et al., 2019), are selected to further verify the influence of coal combustion. Some discussion has been added in the revised manuscript.

Line 320–322, “*In addition, several nitrated phenols, which are abundant in fresh coal combustion flue gas (Lu et al., 2019), also showed similar trends with  $\text{SO}_2$  and PONs (Fig. S5), indicating the potential effect of coal combustion on the concentrations of PONs.*”



**Figure S5.** Time series of PONs, SO<sub>2</sub>, 4-nitrophenol (4NP), and 5-nitrosalicylic acid (5NSA) at the DY site in winter.

Page 9, Line 330: The association of organic nitrate with the inorganic components in the particle phase does not necessarily establish any causal relationships. If it is the salting in effect as proposed by the authors, please provide some quantitative evidence.

**Response:** the salting in effect is cited from by Xu et al. (2015a) as we mentioned on Line 331 in the original manuscript. Our speculation is based on the similar properties of the target compounds and is put forward to provide a possible explanation. However, at present there is no feasible method to quantify the salting-in effect on PONs uptake. The related description has been removed in the revised manuscript.

Page 9, Line 360-365: Again, a positive correlation of RHs with organic nitrates in the particle phase does not necessarily establish any causal relationship. High RHs may just simply promote the photochemistry by generating more OH radicals, or high RHs is likely associated with a pollution episode. Keep in mind that the deliquescence RHs for various inorganic components in the particle phase are essential in determining the aerosol water content and its role in dissolving more water-soluble compounds (caution that some organic nitrates investigated in this study are not considered highly water soluble).

**Response:** the time series of RH and PONs have been shown in Figure S8. The possibility that the increased concentration of PONs was caused by OH enhancement or pollution events can be generally ruled out by the stable ozone and PM<sub>2.5</sub> concentrations. In our other filed measurements, a considerable concentration of MHN125 was found in cloud water samples, and thus the monoterpene-derived PONs is assumed to be soluble to a certain degree. The following discussion has been added in the revised manuscript.

Line 402–403, “At the GZ site, the concentrations of gaseous pollutants and PM<sub>2.5</sub> were generally unchanged during the sampling periods, with no distinct pollution events.”

Line 406–411, “As the humidity increased, the fine particles were primarily in a liquid-like state during the daytime (Slade *et al.*, 2019), and the secondary organic material was likely in aqueous phase when the humidity was higher than 60% (Song *et al.*, 2015). In addition, when the ambient humidity was higher than the deliquescence points of inorganic components (40%-80%) (Martin, S. T, 2000), the emerging liquid water would affect the gas-aqueous partition and increase the heterogeneous uptake of precursors, oxidants, and products (Wang *et al.*, 2017).”

Line 412–414, “It is possible that the epoxides undergo reasonably fast acid-catalyzed reactions at typical SOA acidities and produce a variety of organic nitrate species by nucleophilic reactions with nitrate (NO<sub>3</sub><sup>-</sup>) (Mael *et al.*, 2015), especially during daytime when the acidity of aerosols is strong (Behera *et al.*, 2013).”

Page 18, Figure 2: In addition to the proportion of each organic nitrate species, please also show the total OM mass at different sampling sites.

**Response:** the total OM mass concentrations have been added in Table 3.

Page 21, Figure 7: Please change the color code for PKN229 and LDKN247. It is hard to differentiate these two species based on the current blue hues.

**Response:** the color codes have been changed.

### References:

Docherty, K. S., and Ziemann, P. J.: Reaction of oleic acid particles with NO<sub>3</sub> radicals: Products, mechanism, and implications for radical-initiated organic aerosol oxidation, *Journal of Physical Chemistry A*, 110, 3567-3577, 10.1021/jp0582383, 2006.

Lu, C., Wang, X., Li, R., Gu, R., Zhang, Y., Li, W., Gao, R., Chen, B., Xue, L., and Wang, W.: Emissions of fine particulate nitrated phenols from residential coal combustion in China, *Atmos. Environ.*, 203, 10-17, 10.1016/j.atmosenv.2019.01.047, 2019.

Perraud, V., Bruns, E. A., Ezell, M. J., Johnson, S. N., Greaves, J., and Finlayson-Pitts, B. J.: Identification of Organic Nitrates in the NO<sub>3</sub> Radical Initiated Oxidation of  $\alpha$ -Pinene by Atmospheric Pressure Chemical Ionization Mass Spectrometry, *Environmental Science & Technology*, 44, 5887-5893, 10.1021/es1005658, 2010.

Rindelaub, J. D., Borca, C. H., Hostetler, M. A., Slade, J. H., Lipton, M. A., Slipchenko, L. V., and Shepson, P. B.: The acid-catalyzed hydrolysis of an  $\alpha$ -pinene-derived organic nitrate: kinetics, products, reaction mechanisms, and atmospheric impact, *Atmospheric Chemistry and Physics*, 16, 15425-15432, 10.5194/acp-16-15425-2016, 2016.