Supporting Information for

Synergetic effect of NH_3 and NOx on the production and optical absorption of secondary organic aerosol formation from toluene photooxidation

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Positive matrix factorization (PMF) is a receptor model and multivariate factor analysis tool (Paatero and Tapper, 1994; Paatero, 1997). Recently, the PMF model was used to provide better separation of different organic components through high-resolution (HR) mass spectra data (Liu et al., 2014). This model was expressed as below:

$$x_{ij} = \Sigma_p g_{ip} f_{pj} + e_{ij}$$

where i and j refer to values of j species in i samples, respectively, p is the number of factors, and used a least-squares fitting process, minimizing a quality of fit parameter.

In our study, CU AMS PMF Execute Tool v 3.04A, which was developed by Ulbrich et al. (Ulbrich et al., 2009), was used for the PMF analysis. High-resolution ion fragments at m/z from 12-160 were used. We generated the organic data matrices and the corresponding error matrices from PIKA v 1.15D. Ions were classified and down-weighted according to the signal-to-noise ratios (SNR). $0.2<SNR<2$ was classified as the weak ions and down-weighted by a factor of 2, $SNR<0.2$ was bad ions and removed from the analysis. ince O^+, HO^+, H_2O^+ and CO^+ are related proportionally only to CO_2^+ in the fragmentation table, the error values for each of these m/z were multiplied to avoid excessive weighting of CO_2^+. The data were analyzed using the PMF2 algorithm (Paatero et al., 2002) with fpeak varying between -1 and 1.

A summary of the PMF results is presented in Fig. S1-S3. After an extensive evaluation of the mass spectral profiles and time series of different number of factors and the rotational forcing parameter, fPeak, the 2-factor solution with fPeak = 0 was chosen for toluene SOA. The OA components of the 2-factor solution solved under different fPeak values show very similar mass spectral patterns.

The direct comparisons of the mass spectra and time series of 3-factor solution are shown in Fig. S4. The 3-factor solution splits the High-nitrogen OA (Hi-NOA) into two components for which we cannot offer a physically meaningful interpretation. While the results of 2-factor solution are also used in the familiar chamber study(Chen et al., 2021; Chen et al., 2019). We therefore choose the 2-factor solution.

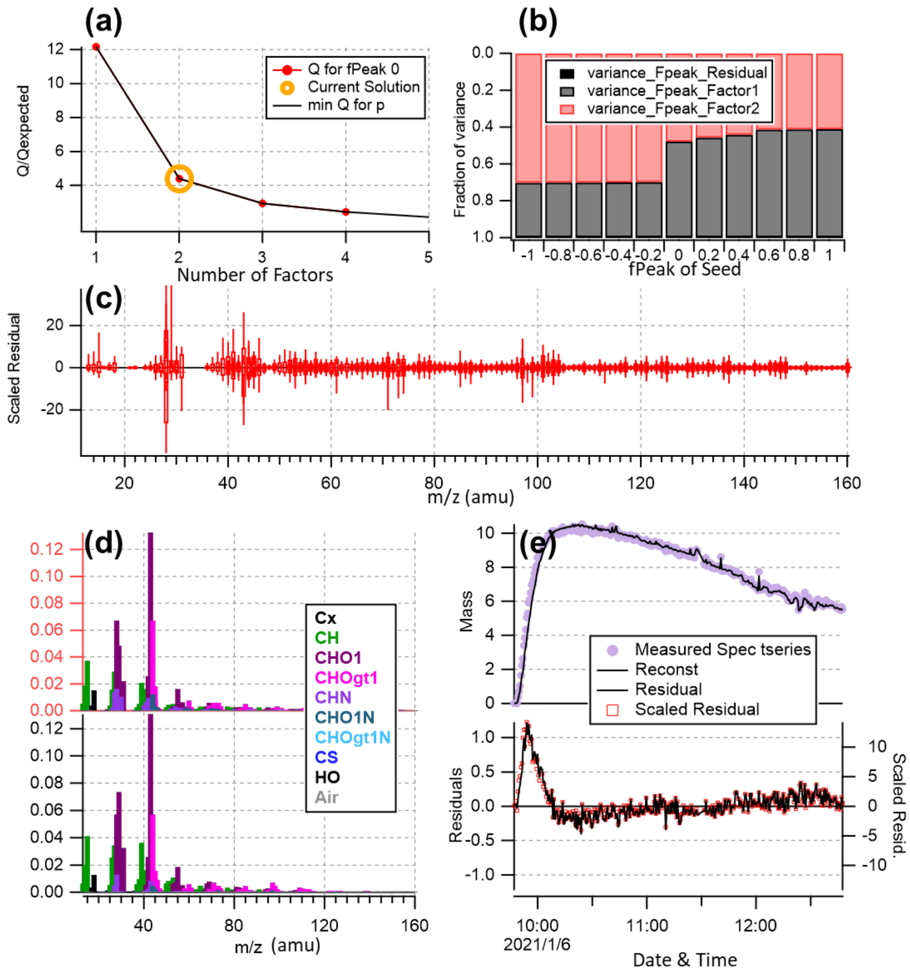

Fig. S1 The 2-factor solution for the toluene OH-oxidation in the presence of NH_3.

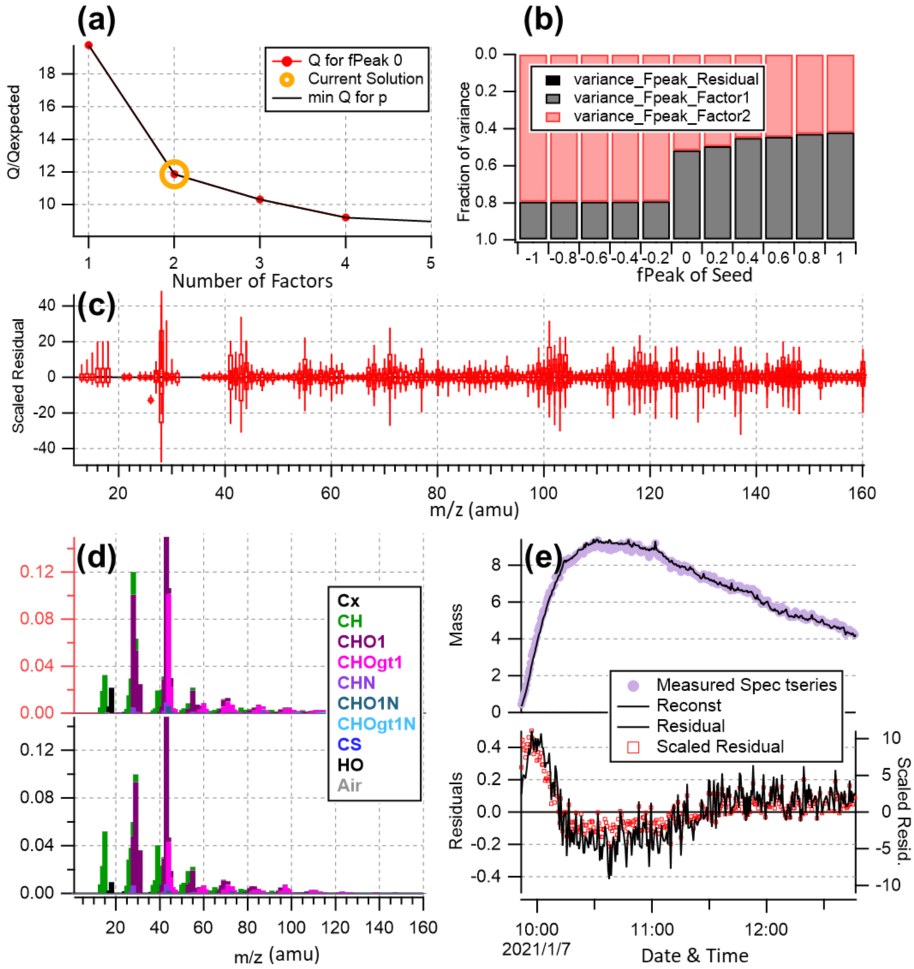

Fig. S2 The 2-factor solution for the toluene OH-oxidation in the presence of NOx.

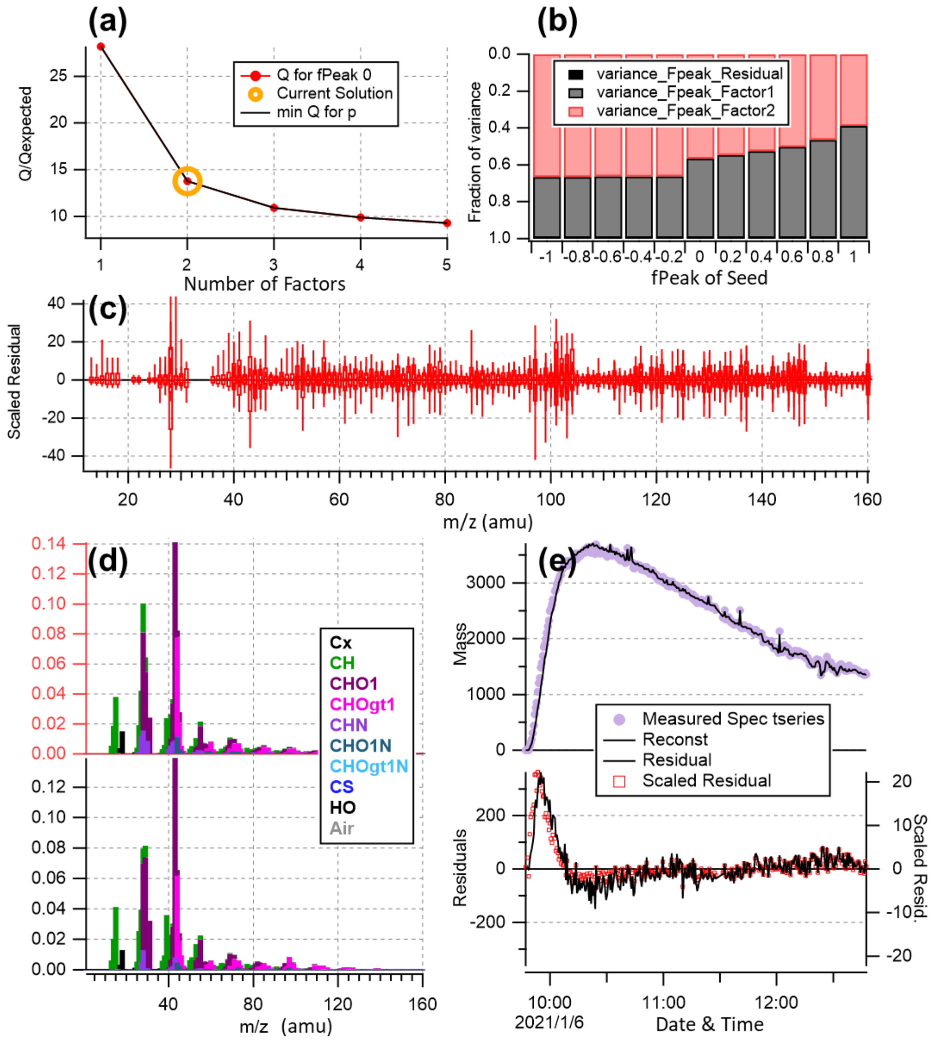

Fig. S3 The 2-factor solution for the toluene OH-oxidation in the presence of both NOx and NH_3.

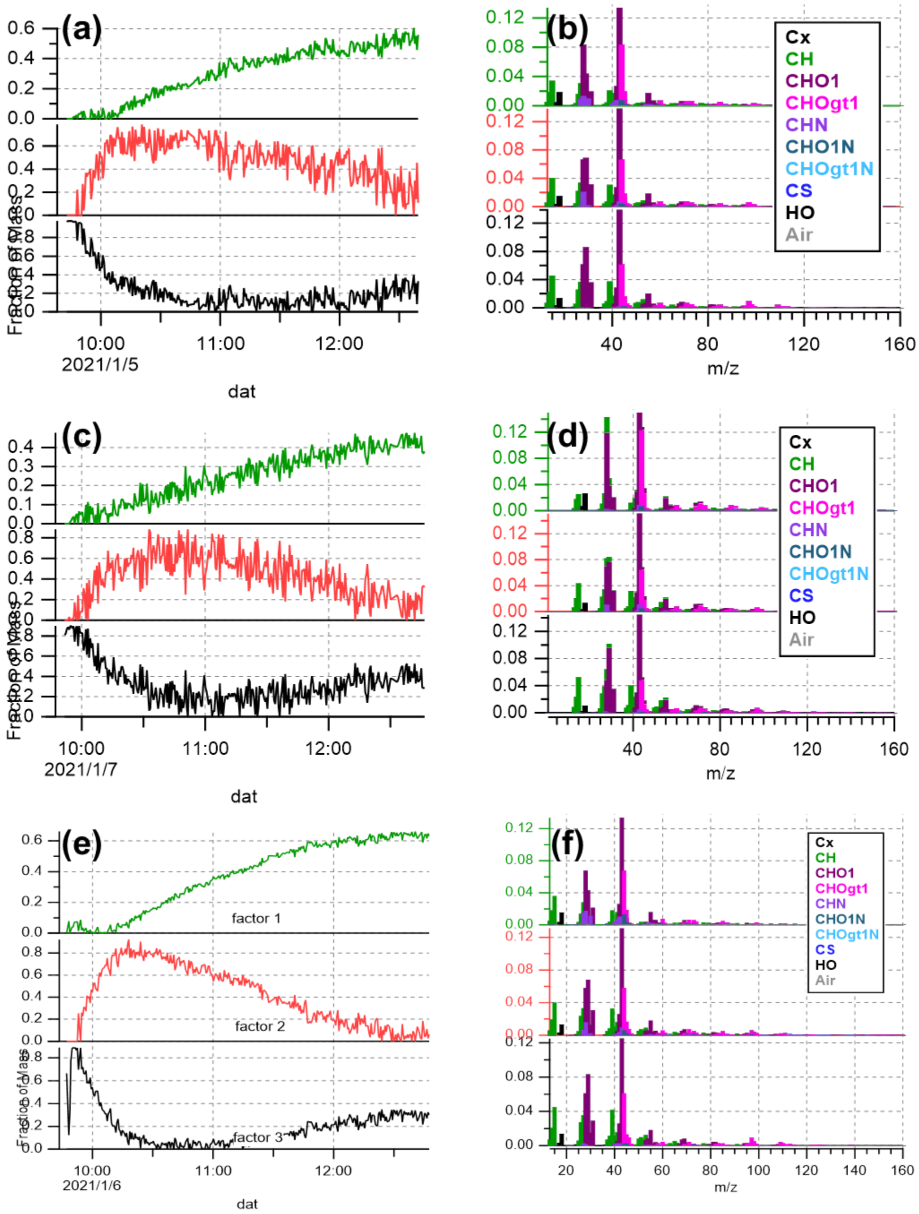

Fig. S4 (a), (c), and (e): High resolution mass spectra 3-factor solution for the Exp.2, 3, and 4, respectively. (b), (d), and (f): Time series of mass concentration of OA in each factor.

Reference:

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