Supplement of

Hygroscopicity of organic compounds as a function of organic functionality, water solubility, molecular weight and oxidation level

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S1. Schematic of the HTDMA system.

The principle of HTDMA can be described as follow: the generated aerosol particles passed through a silica diffusion dryer and a Nafion dryer (Perma Pure, MD-700-24S-3), and were dried to RH < 8 %. Subsequently, the dried particles were neutralized and obtained Boltzmann charge distribution by using a Kr85 neutralizer (TSI Inc.). After charging, the monodisperse aerosols with specific diameters were selected by the first differential mobility analyzer (DMA1, Model 3081L, TSI Inc.). Afterwards, the monodisperse aerosol particles entered into a Nafion humidifier (Perma Pure, PD-100T-24MSS) with a residence time about 2.7s, and they were humidified to a given RH (10-90 %). After humidifying, there was a similar system including another DMA (DMA2, Model 3081L, TSI Inc.) and a condensation particle counter (CPC, Model 3772, TSI Inc.) to measure the number size distribution of the humidified particles. The whole experiment system was controlled by air conditioning with the room temperature of around 24 ℃, and the internal temperature was kept at ±0.5K around the standard value. It should be noted that, because of we just measure the mode value of GF distribution of humidified particles, the multiple charge correction was ignored (Tan et al., 2013).

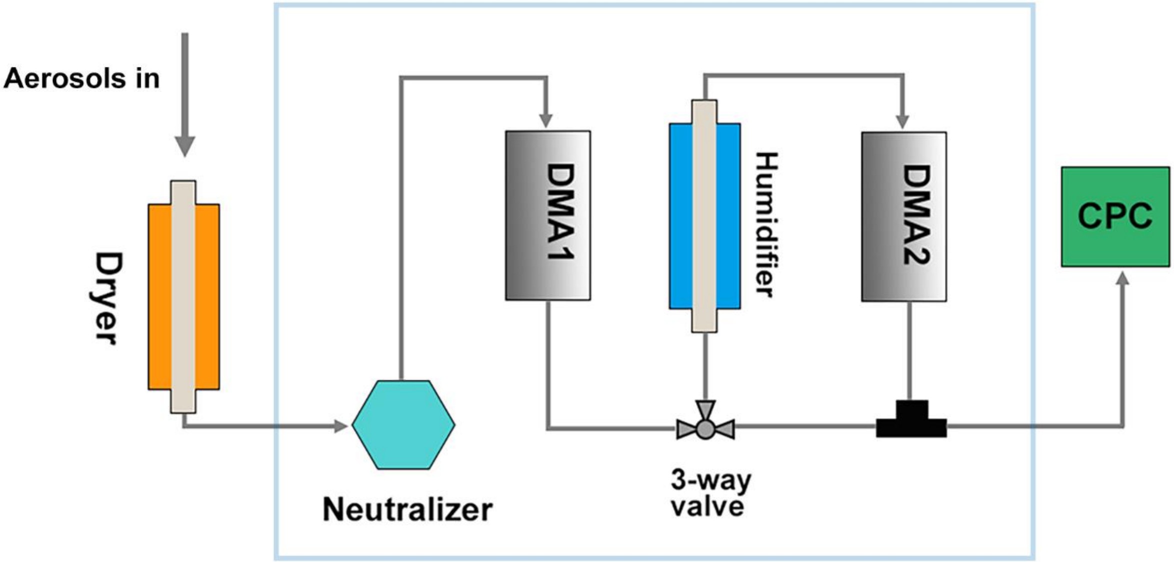

Figure S1. A schematic of the HTDMA instrument system.

S2. Calibration measurements of HTDMA by using ammonium sulfate (AS)

To show the measured hygroscopic data is agree well with the E-AIM predictions and as well as previous studies, and the deliquescence RH is around 78 %. Therefore, our HTDMA is accurate according to the calibration result of ammonium sulfate, in addition, The GF uncertainty of instrument system is ±0.5 %, and the measured GF at given RH are the average values of 5 times measurements, within the corresponding standard deviation less than 0.03.

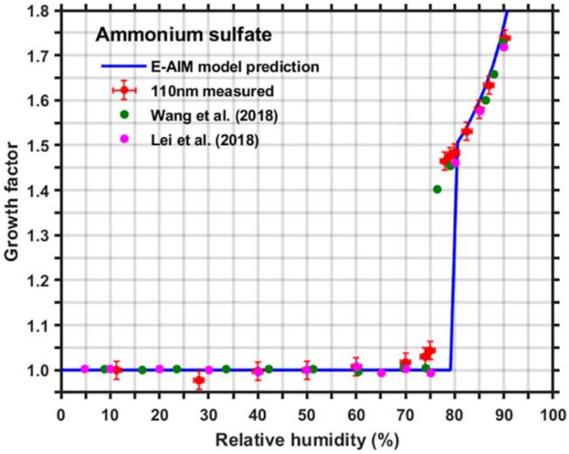

Figure S2. Hygroscopic growth factors of 110nm ammonium sulfate, and the blue line represents the E-AIM predictions. The green and magenta dots indicate the GFs of ammonium sulfate from Wang et al. (2018) and Lei et al. (2018), respectively.

S3. Input setting and calculations for E-AIM and UmanSysProp

In E-AIM, RH was varied between 5 % to 90 % and GF values of the pure component was calculated as Eq. (1) (Wang et al., 2018):

$$GF = \left[1 + \frac{n_w M_w/\rho_w}{\sum_i (m_i/\rho_i)}\right]^{\frac{1}{3}}, \tag{1}$$

where M_w is the molar mass of water, ρ_w is the density of water, m_i and ρ_i are the mass and density of the pure component i, n_w is the mole number of water at a certain RH. In UManSysProp, molecular subgroups were converted according to their Simplified Molecular Input Line Entry System (SMILES) and the input setting of RH was varied between 50 to 99 % (Topping et al., 2016).

S4. For slightly soluble organics, hygroscopicity parameter, κ various with RHs.

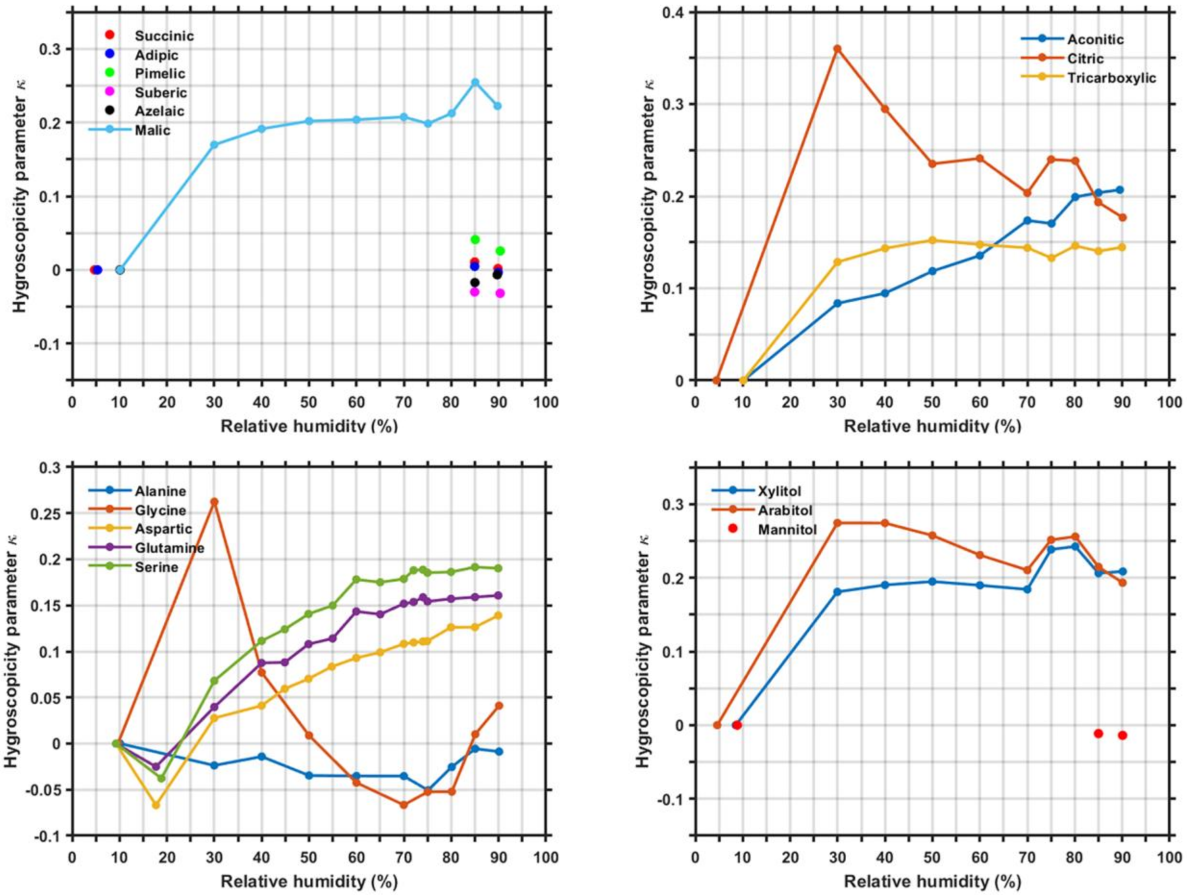

Figure S3 Hygroscopicity parameter, κ of organic components at different RHs (initial dry diameter of 200 nm at RH < 10 %).

References

Lei, T., Zuend, A., Cheng, Y., Su, H., Wang, W., and Ge, M.: Hygroscopicity of organic surrogate compounds from biomass burning and their effect on the efflorescence of ammonium sulfate in mixed aerosol particles, Atmos.Chem.Phys., 18, 1045, https://doi.org/10.5194/acp-18-1045-2018, 2018.

Tan, H. B., Xu, H. B., Wan, Q. L., Li, F., Deng, X. J., Chan, P. W., Xia, D., and Yin, Y.: Design and Application of an Unattended Multifunctional H-TDMA System, Journal of Atmospheric and Oceanic Technology, 30, 1136-1148, 10.1175/Jtech-D-12-00129.1, https://doi.org/10.1175/JTECH-D-12-00129.1, 2013.

Topping, D., Barley, M., Bane, M. K., Higham, N., Aumont, B., Dingle, N., and McFiggans, G.: UManSysProp v1. 0: an online and open-source facility for molecular property prediction and atmospheric aerosol calculations, Geoscientific Model Development, 9, 899-914, https://doi.org/10.5194/gmd-9-899-2016, 2016.

Wang, Z., Jing, B., Shi, X., Tong, S., Wang, W., and Ge, M.: Importance of water-soluble organic acid on the hygroscopicity of nitrate, Atmos. Environ., 190, 65-73, https://doi.org/10.1016/j.atmosenv.2018.07.010, 2018.