

1 *Supplement of*
2 **Predictions of the glass transition temperature and viscosity of**
3 **organic aerosols by volatility distributions**

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19 **Training dataset**

20 To develop Equations (1) and (2), total 2325 organic compounds are included
21 in the training dataset. 42 CH compounds, 259 CHO compounds and 35 CHON
22 compounds have measured T_g values (Koop et al., 2011; Rothfuss and Petters, 2017;
23 Lessmeier et al., 2018). 1154 compounds including 391 CH, 524 CHO and 239 CHON
24 compounds with both measured melting temperatures (T_m) and measured pure
25 compound saturation mass concentrations (C^0) (Table S1) are adopted from the
26 MPBPWIN Program Test Sets (<http://esc.syrres.com/interkow/EpiSuiteData.htm>)
27 included in the Estimation Programs Interface (EPI) Suite software version 4.1. T_g of
28 these compounds are estimated from measured T_m applying the Boyer-Kauzmann rule:
29 $T_g = g \cdot T_m$ with $g = 0.7$ (Koop et al., 2011). This rule has been validated providing good
30 estimates of T_g (Koop et al., 2011). Measured T_g , T_m or C^0 for CHOS compounds are
31 sparse and we adopt 835 CHOS compounds included in Li et al. (2016) with their T_m
32 and C^0 estimated by the EPI Suite software (Table S1). Estimation limitations exist in
33 EPI Suite, for example, the disagreement between measured and estimated C^0 increases
34 as the vapor pressure decreases below 10^{-4} Pa (Li et al., 2016), which may affect the T_g
35 predictions for compounds with low volatility. However, given the large measured data
36 points included in the training data set, the estimation bias introduced by the EPI Suite
37 may not largely impact the accuracy of Eqs. (1) and (2), as indicated by the good
38 predictions for the T_g of the testing data set (Fig. 1c).

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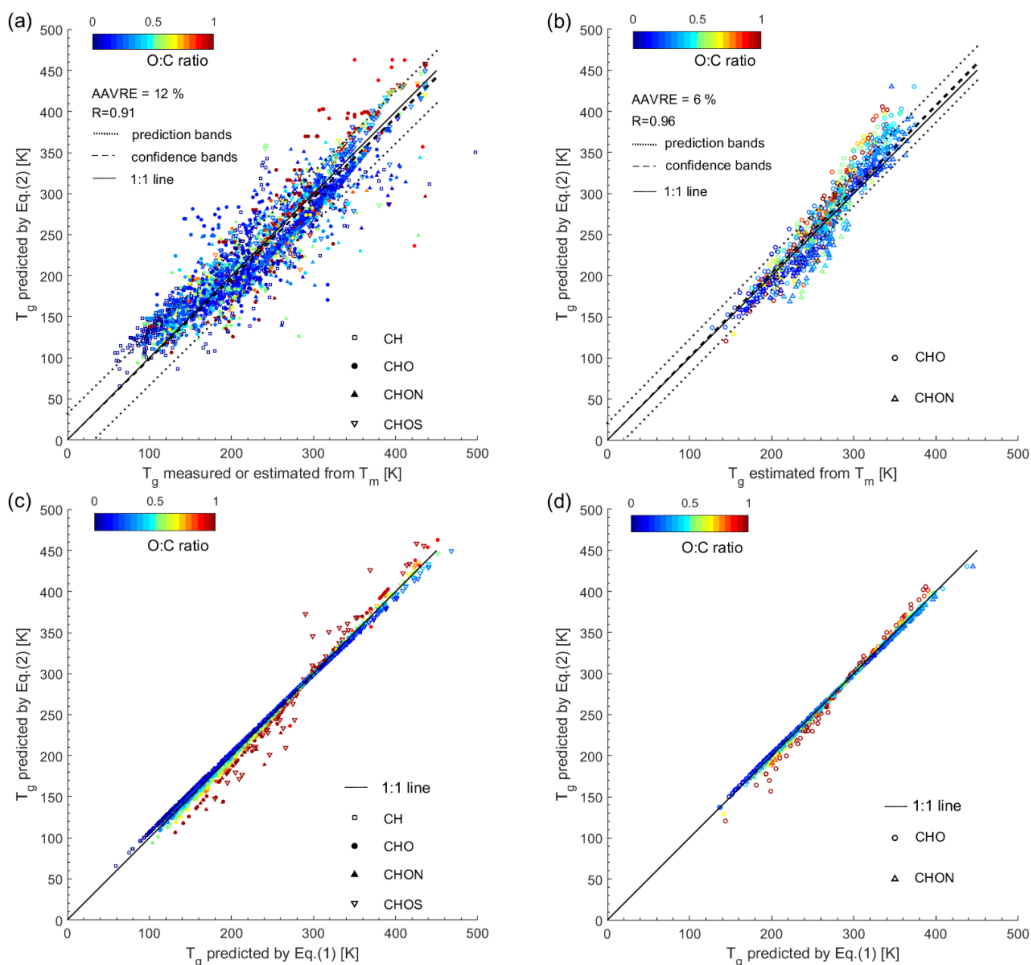


Figure S1. Predicted T_g for compounds shown in Fig. 1a using Eq. (2) developed in this study compared to (a) measured and estimated T_g by the Boyer-Kauzmann rule and (c) predicted T_g using Eq. (1). Predicted T_g for SOA components (Shiraiwa et al., 2014) using Eq. (2) compared to (b) estimated T_g by the Boyer-Kauzmann rule and (d) predicted T_g using Eq. (1). The markers are color-coded by atomic O:C ratio. The dashed and dotted lines in (a) and (b) show 68% confidence and prediction bands, respectively. The solid line shows the 1:1 line.

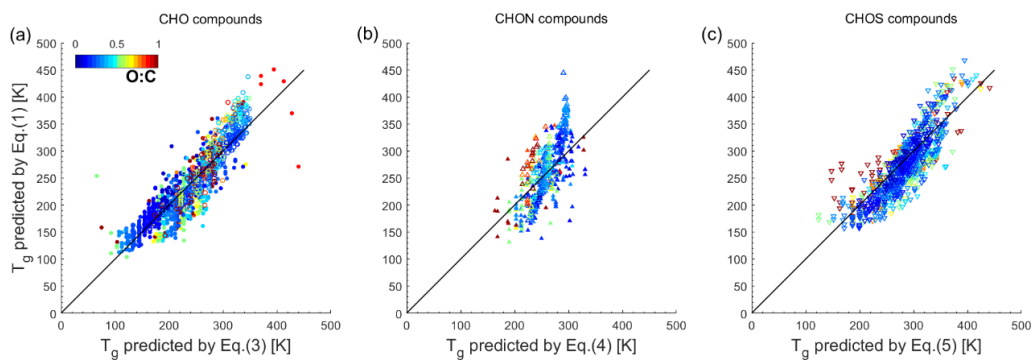


Figure S2. Predicted T_g using Eq. (1) compared to predicted T_g using (a) Eq. (3) for CHO compounds, (b) Eq. (4) for CHON compounds, and (c) Eq. (5) for CHOS compounds. The solid line shows the 1:1 line. The markers are color-coded by the atomic O:C ratio.

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