Supplement of

Predictions of the glass transition temperature and viscosity of organic aerosols from volatility distributions

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Table S1. Number of the compounds included in the training dataset and their T_g, C^0 and T_m measured or otherwise estimated.

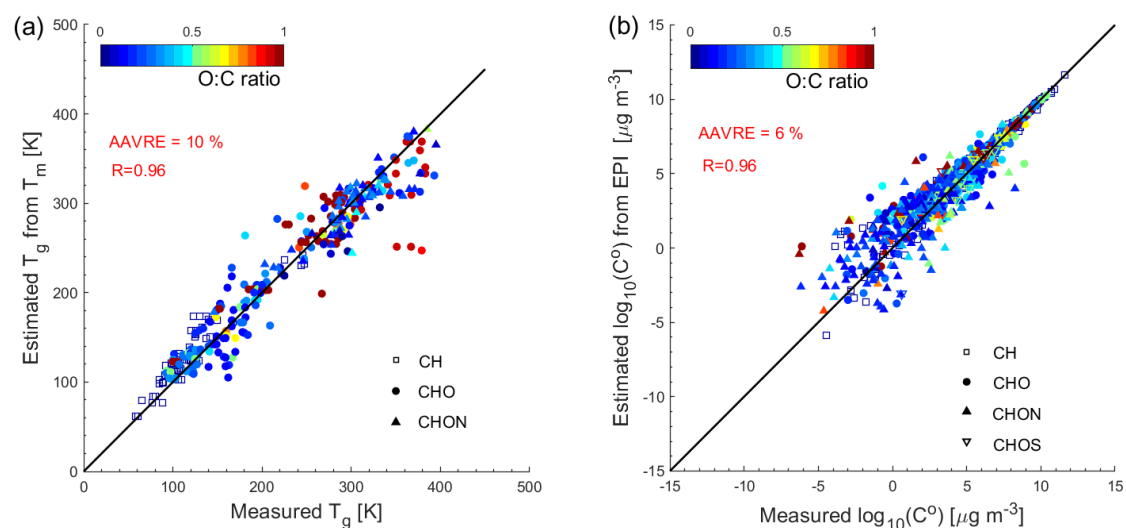|	CH	CHO	CHON	CHOS
Both T_g and C^0 measured	38	125	5	0
Measured T_g, C^0 estimated from EPI Suite	4	134	30	1
T_g estimated from measured T_m, measured C^0	391	537	241	18
T_g estimated from T_m, T_m estimated from EPI Suite, measured C^0	0	0	0	11
T_g estimated from measured T_m, C^0 estimated from EPI Suite	0	0	0	63
T_g estimated from T_m, T_m and C^0 estimated from EPI Suite	0	0	0	850

Figure S1. (a) Comparison of the measured T_g (Koop et al., 2011; Dette et al., 2014; Rothfuss and Petters, 2017; Lessmeier et al., 2018; Zhang et al., 2019) and the T_g estimated by the Boyer–Kauzmann rule for 336 organic compounds with their measured T_m available. (b) Comparison of pure compound saturation mass concentration (C^0) measured and estimated from the EPI suite for 1637 organic compounds included in the training dataset.
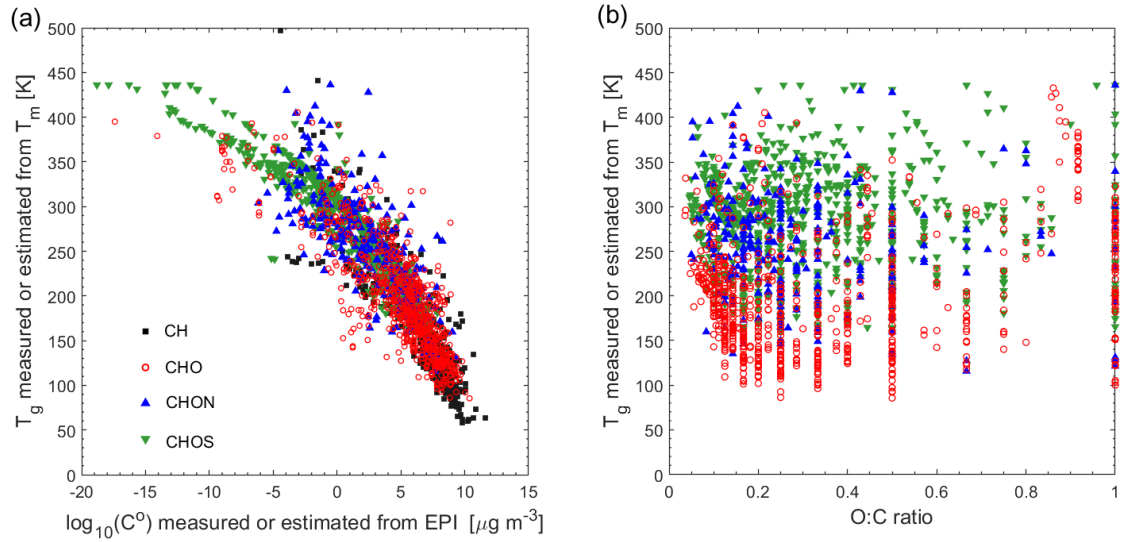
Figure S2. T_g of organic compounds in the training dataset plotted against (a) pure compound saturation mass concentration (C^0) and (b) the atomic O:C ratio.
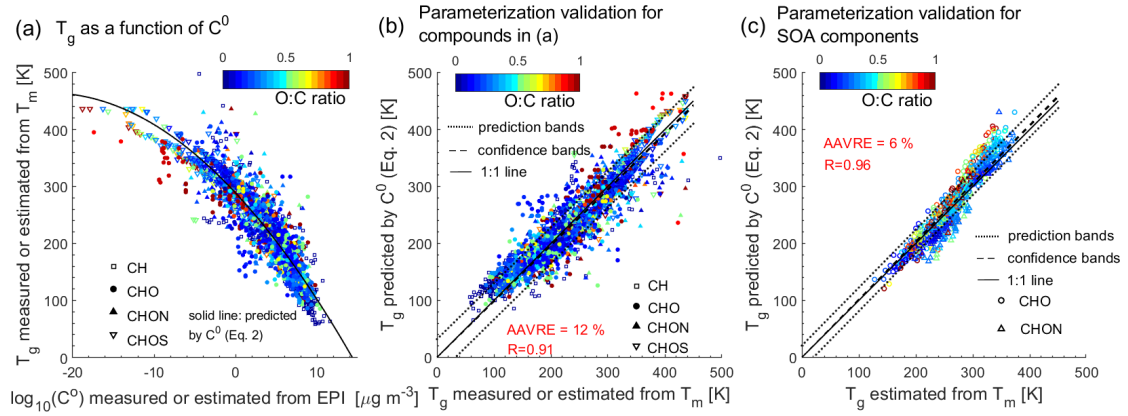

Figure S3. (a) T_g of organic compounds in the training dataset plotted against C^0. The solid line shows the predictions of T_g by C^0 (Eq. 2). (b) Predicted T_g by C^0 (Eq. 2) for compounds shown in (a) compared to measured or otherwise estimated T_g from T_m. (c) Predicted T_g for SOA components (Shiraiwa et al., 2014) using Eq. (2) plotted against estimated T_g from T_m with the Boyer-Kauzmann rule. The correlation coefficient (R) and the average absolute value of the relative error (AAVRE) are shown. The dashed and dotted lines in (b) and (c) show 68% confidence and prediction bands, respectively.
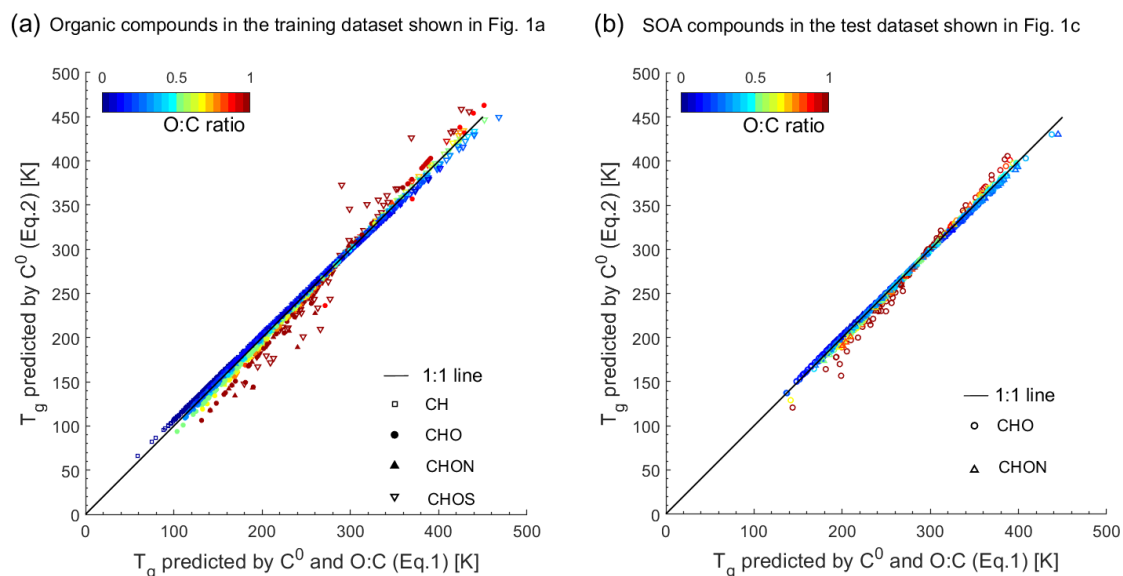
Figure S4. T_g predicted as a function of C^0 using Eq. (2) compared to T_g predicted as a function of C^0 and the O:C ratio using Eq. (1) for (a) organic compounds included in the training dataset and (b) SOA components (Shiraiwa et al., 2014) in the test dataset.
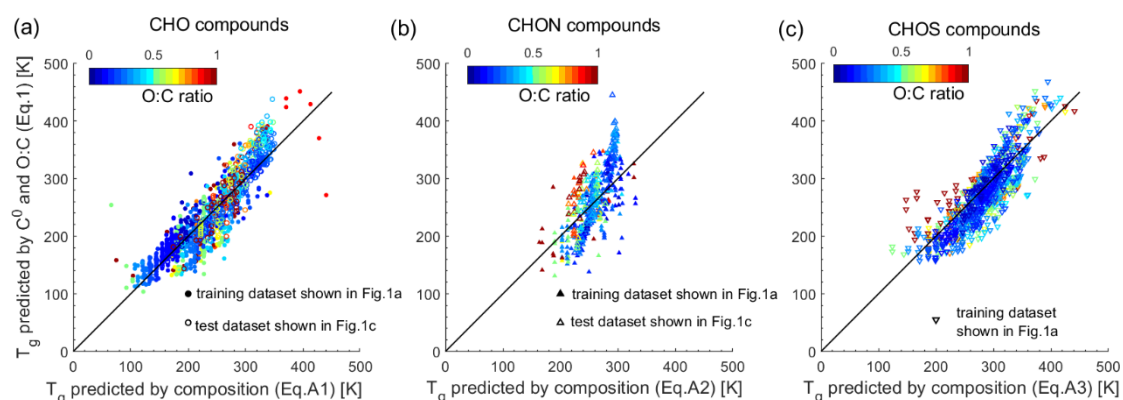

Figure S5. T_g predicted as a function of C^0 and the O:C ratio using Eq. (1) compared to T_g predicted as a function of elemental compositions using (a) Eq. (A1) for CHO compounds, (b) Eq. (A2) for CHON compounds, and (c) Eq. (A3) for CHOS compounds. The solid line shows the 1:1 line.

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