Desorption Lifetimes and Activation Energies Influencing Gas-Surface Interactions and Multiphase Chemical Kinetics

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This Supplement comprises of seven figures (S1-S7).

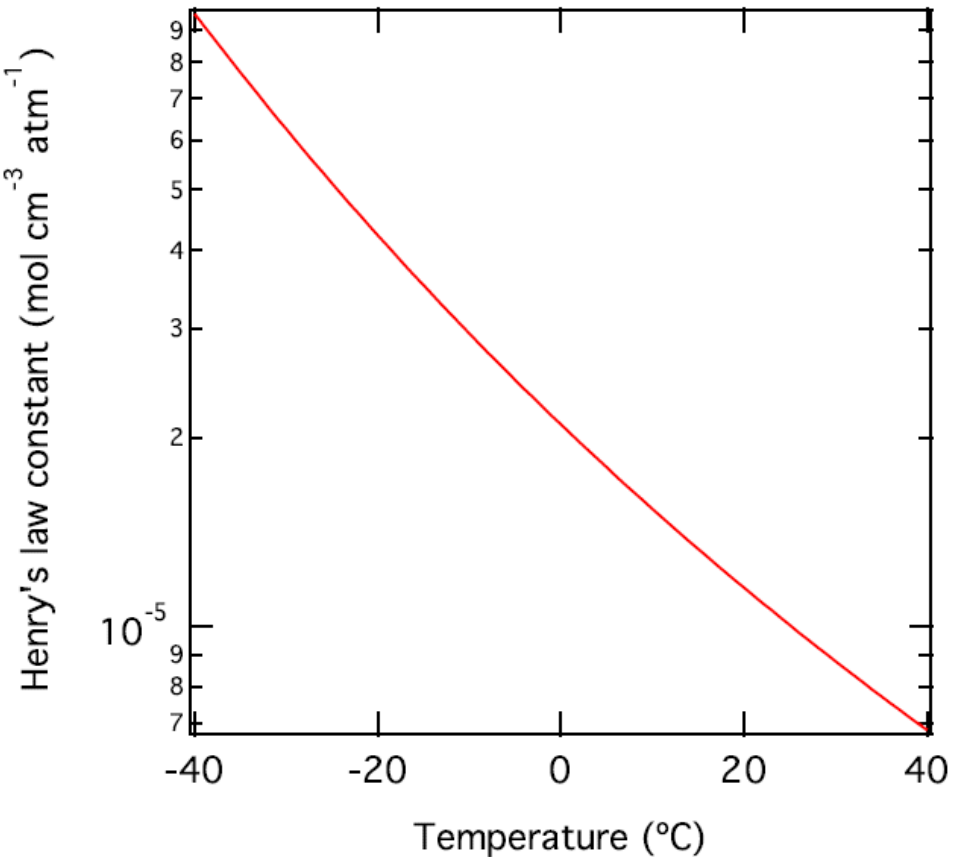

Figure S1. The temperature dependence of the Henry's law coefficient is shown using the van't Hoff equation with solvation enthalpy of 20 kJ mol^{-1}.

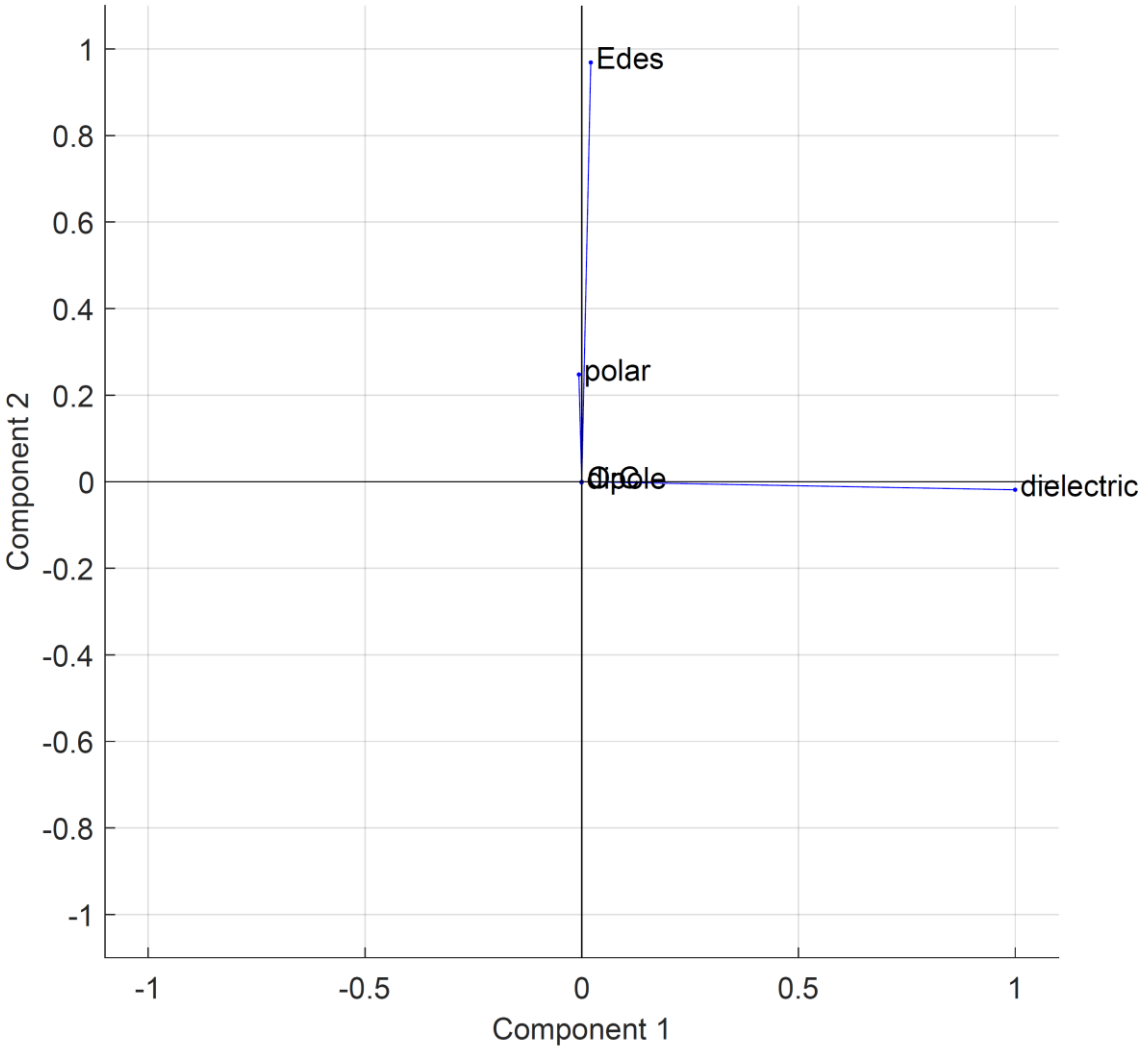

Figure S2. Coefficients derived from principal component analysis to examine the dependencies between the desorption energy (E_{des}^{0}), polarizability (polar, α), dipole moment (dipole, μ), oxygen to carbon ratio ($O{:}\,C$), and relative permittivity of the substrates (dielectric, ε_r).

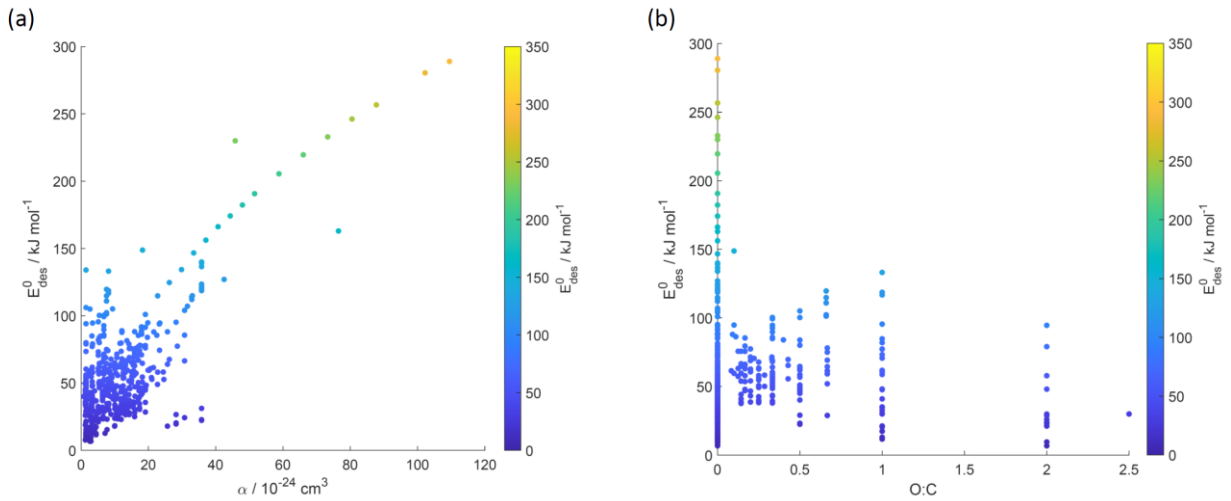

Figure S3. Desorption energy (E^0_{des}) as a function of gas species polarizability (α) in panel (a) and as a function of oxidation state of gas species expressed as $O{:}C$ (b) using data from Tables A1-A15. Panels (a) and (b) reflect data from Fig. 8.

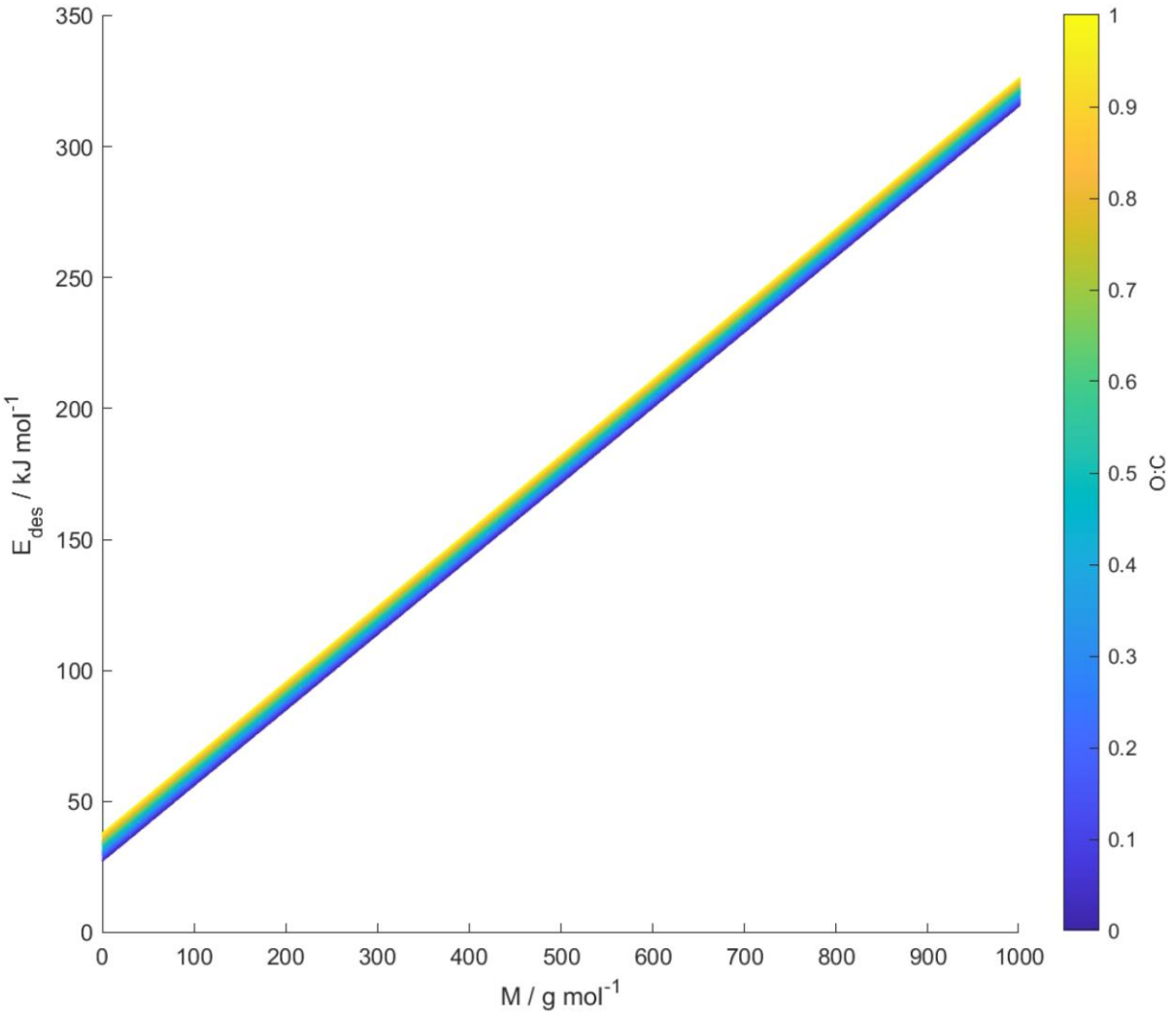

Figure S4. E^0_{des} values derived from the new parameterization (Eq. (16)) applying arbitrary values of molar mass (M) and $O{:}C$, the latter coded as symbol color described by the color bar.

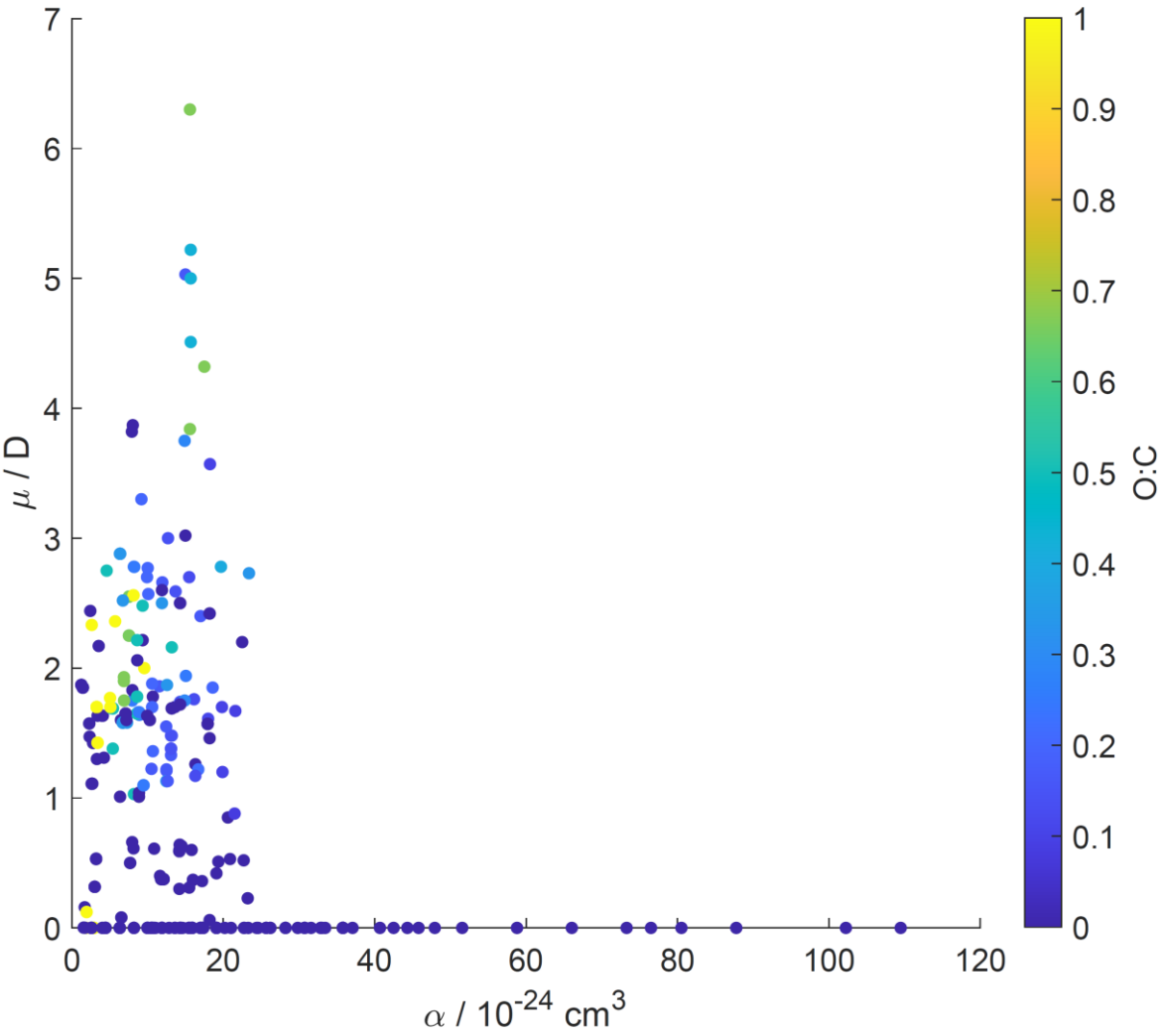

Figure S5. The dipole moment (μ) is plotted against the polarizability (α) where color shading indicates the oxidation state ($O:C$). Note that three gas species with $O:C > 1$ (CO_2 and formic acid) are included in this plot as having $O:C = 1$ to allow for better visualization of entire data set.

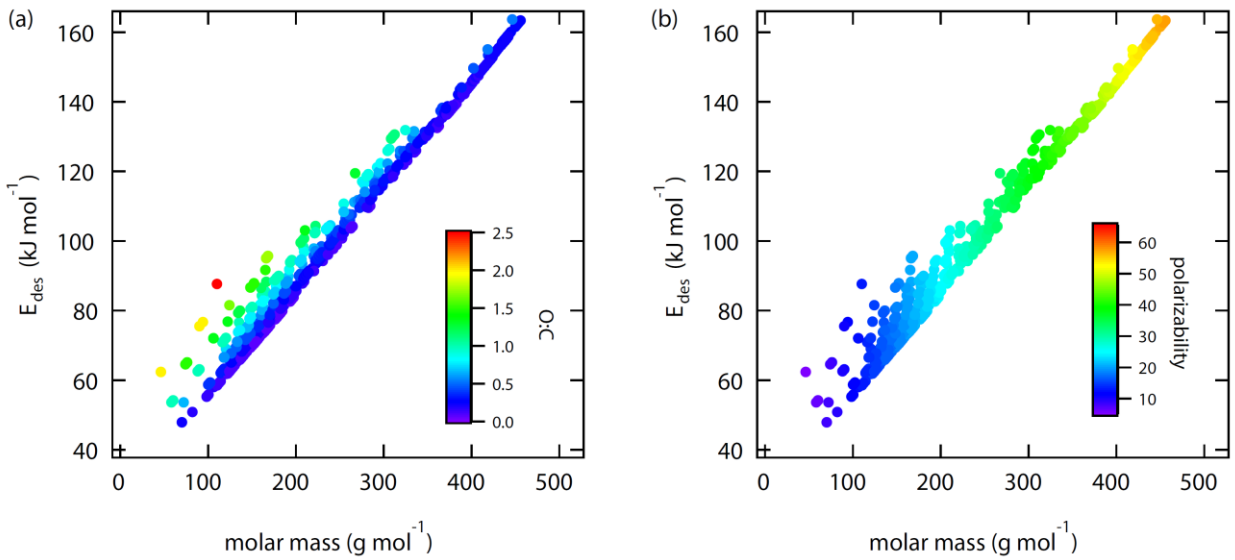

Figure S6. Calculated desorption energies (E^0_{des}) of SOA precursor gases from (Shiraiwa et al., 2014) as a function molar mass and its dependence on $O{:}C$ (a) and polarizability (b) using parameterization Eq. (16).

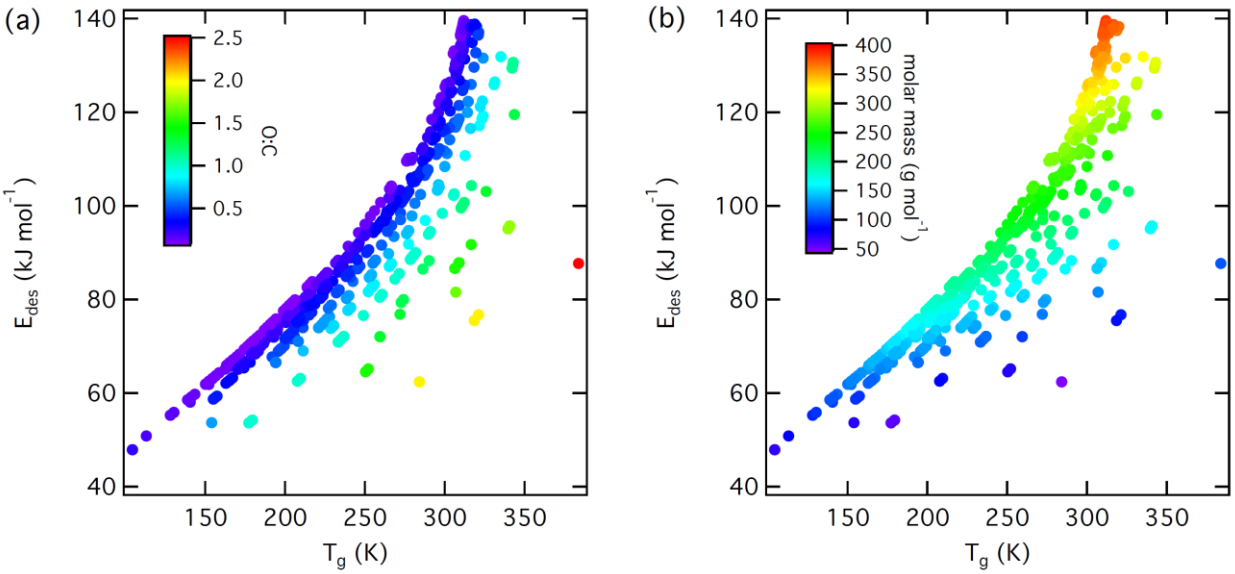

Figure S7. Relationship between calculated desorption energies (E^0_{des}) of SOA precursor gases from (Shiraiwa et al., 2014) and species' glass transition temperature (T_g) and its dependence on $O{:}C$ (a) and molar mass (b) using parameterization Eq. (16).

References

Shiraiwa, M., Berkemeier, T., Schilling-Fahnestock, K. A., Seinfeld, J. H., and Pöschl, U.: Molecular corridors and kinetic regimes in the multiphase chemical evolution of secondary organic aerosol, Atmos. Chem. Phys., 14, 8323-8341, 10.5194/acp-14-8323-2014, 2014.