Supporting information

Evaluation of dipole moment of polyhedral oligomeric silsesquioxane compounds

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Contents:

1. Capacitance and dielectric constant of reference compound

Table S1. Capacitance and dielectric constant of toluene, acetone, methanol, and pure water.

	C [pF]	ε^a [-]	$\varepsilon_{ref}{}^b$ [-]
Toluene	7.7	3.8	2.4
Acetone	49.7	24.2	20.7
Methanol	76.2	37.0	32.7
Water	175.1	85.1	80.1

Measuring conditions; temperature: 25 °C, frequency: 1 kHz, voltage: 1 V, C: measured value of capacitance, ε^a: Measured value of dielectric constant, $\varepsilon_{ref}{}^b$: Reference value of dielectric constant to the solute, and subscript *12* to the solution.

2. α-plot and β-plot

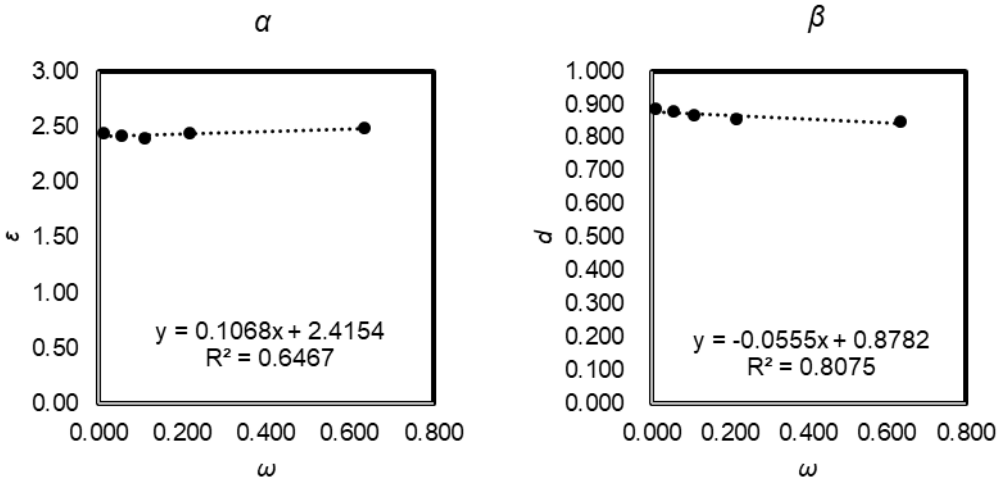

Figure S1. Plot of limonene solution in benzene. (α); dielectric constant to weight fraction, (β); density to weight fraction.

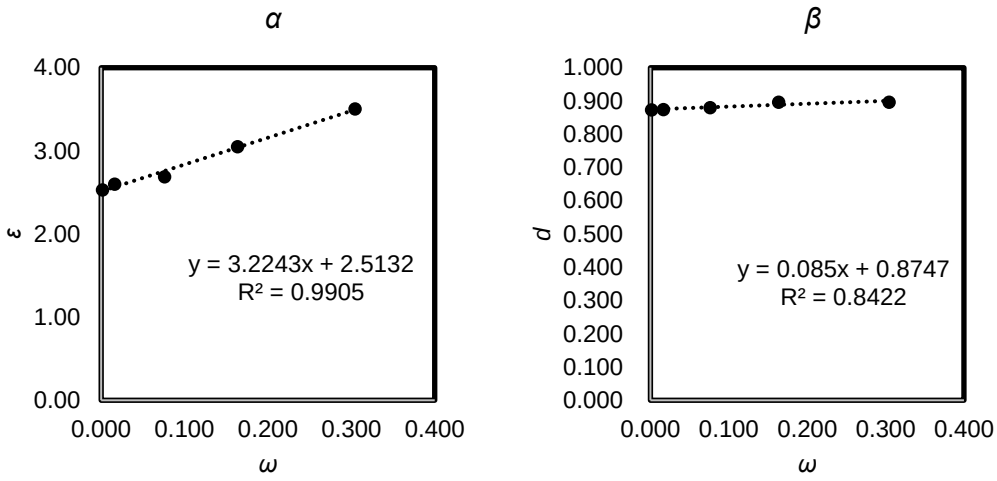

Figure S2. Plot of methylbenzoate solution in benzene. (α); dielectric constant to weight fraction, (β); density to weight fraction.

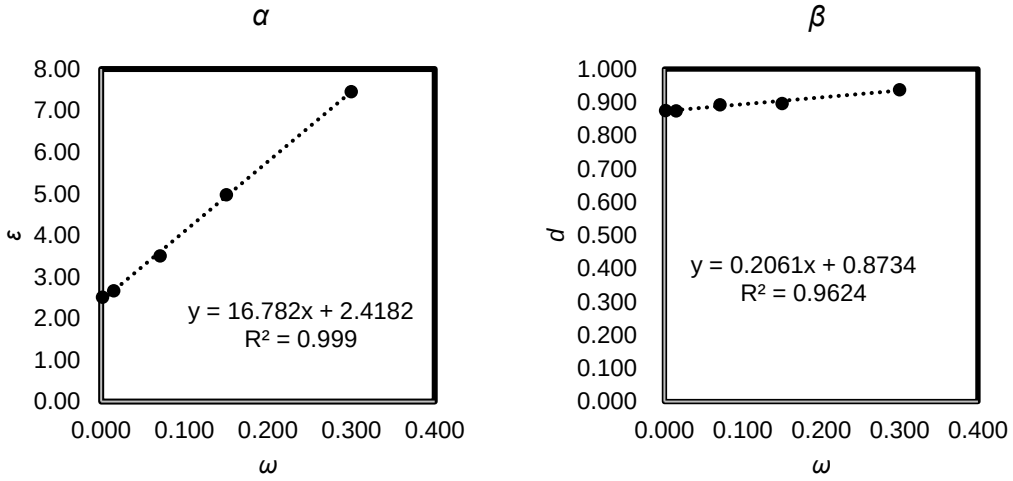

Figure S3. Plot of nitrobenzene solution in benzene. (α); dielectric constant to weight fraction, (β); density to weight fraction.

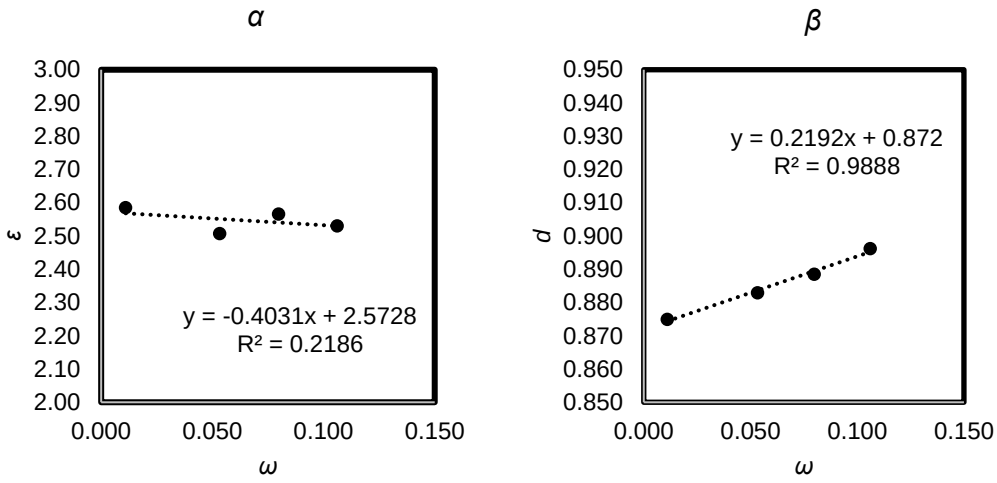

Figure S4. Plot of 7B1Pr-POSS solution in benzene. (α); dielectric constant to weight fraction, (β); density to weight fraction.

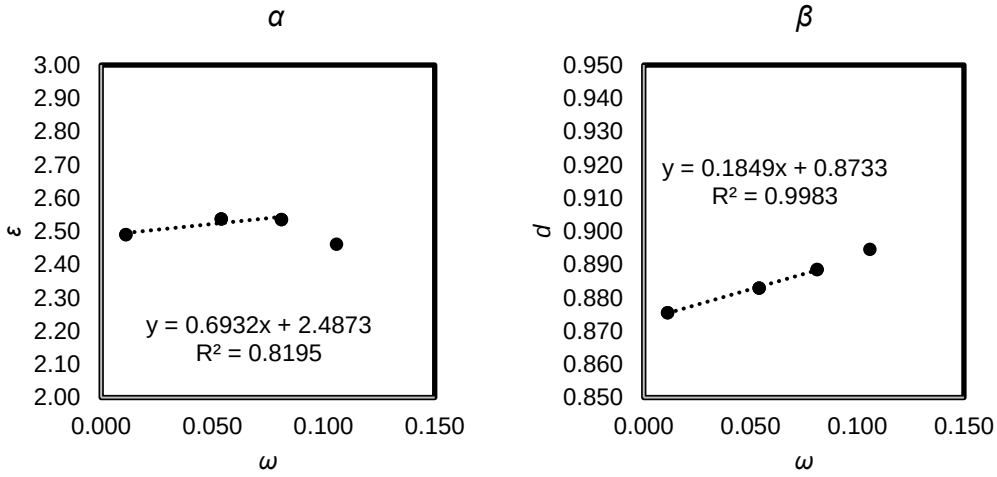

Figure S5. Plot of 7B1AL-POSS solution in benzene. (α); dielectric constant to weight fraction, (β); density to weight fraction.

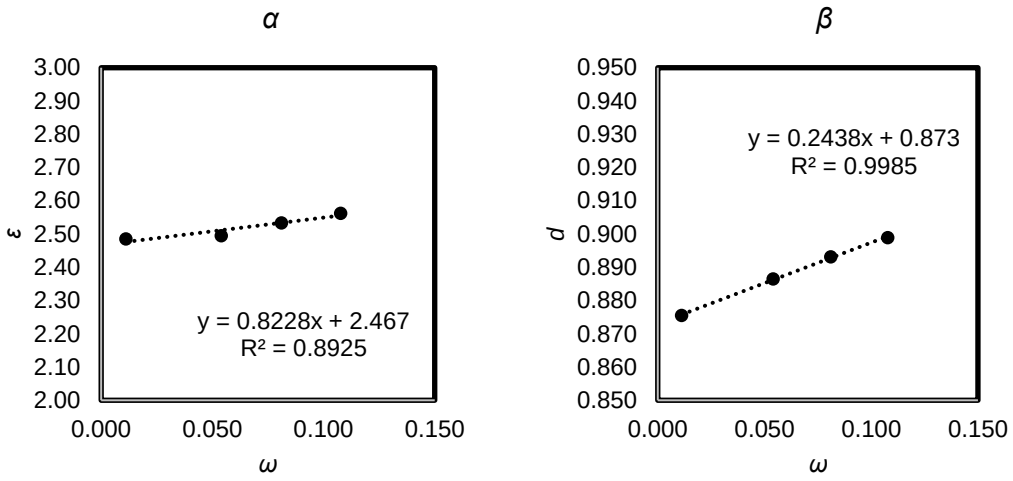

Figure S6. Plot of 7B1NH$_2$-POSS solution in benzene. (α); dielectric constant to weight fraction, (β); density to weight fraction.

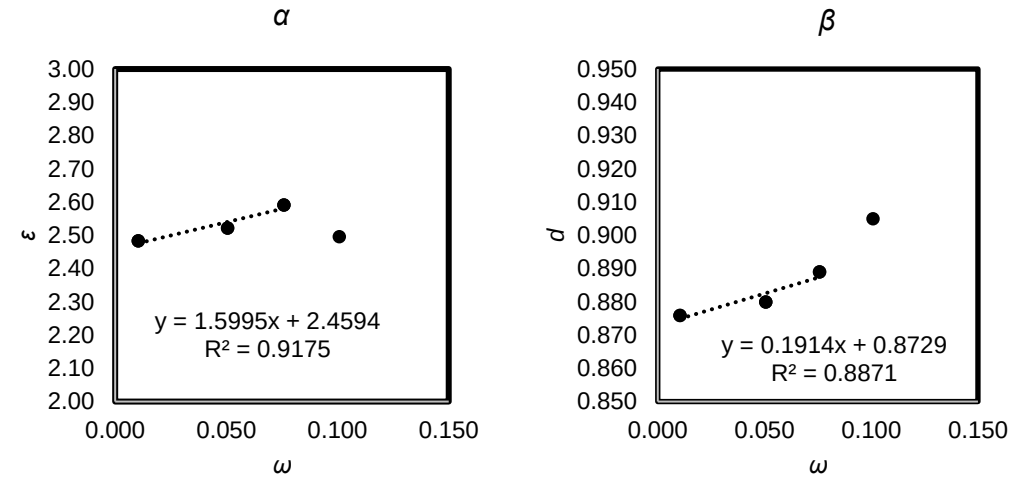

Figure S7. Plot of 7B1Cl-POSS solution in benzene. (α); dielectric constant to weight fraction, (β); density to weight fraction.

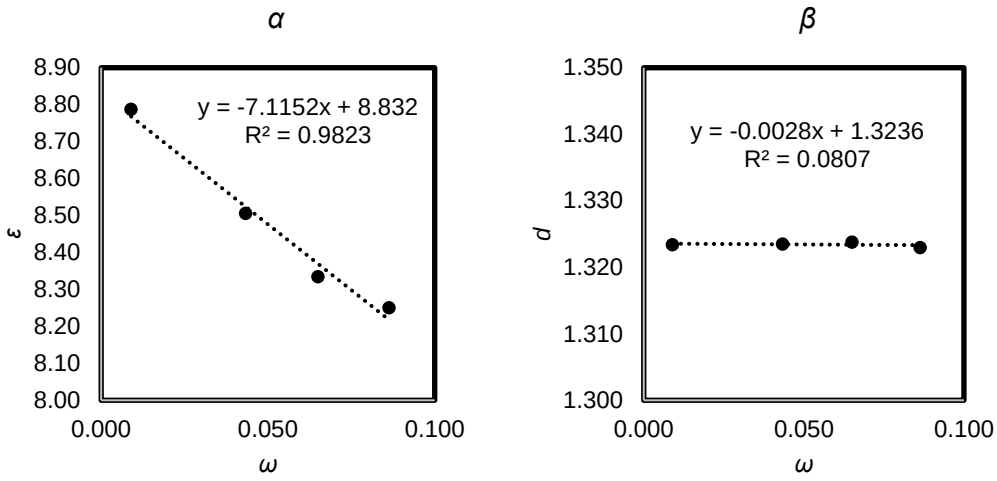

Figure S8. Plot of 7Ph1AL-POSS solution in dichloromethane. (α); dielectric constant to weight fraction, (β); density to weight fraction.

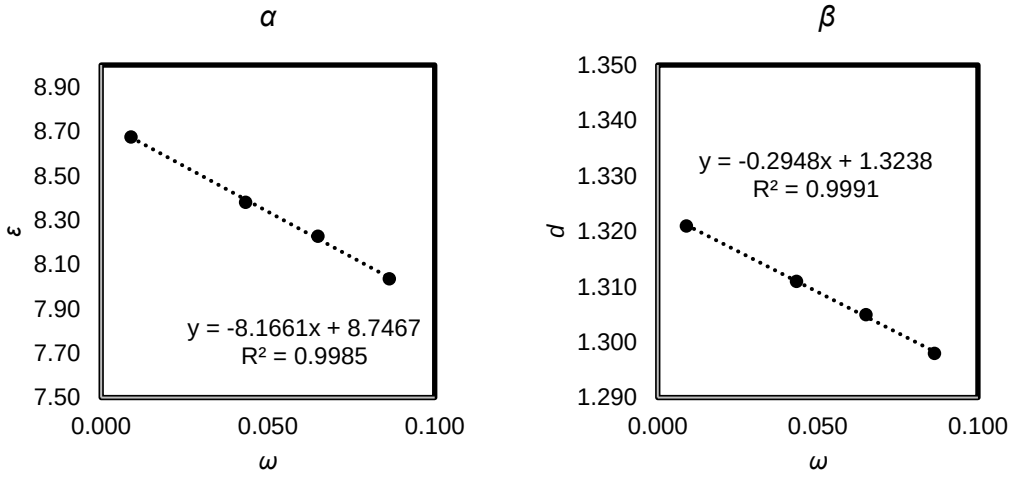

Figure S9. Plot of 7B1AL-POSS solution in dichloromethane. (α); dielectric constant to weight fraction, (β); density to weight fraction.

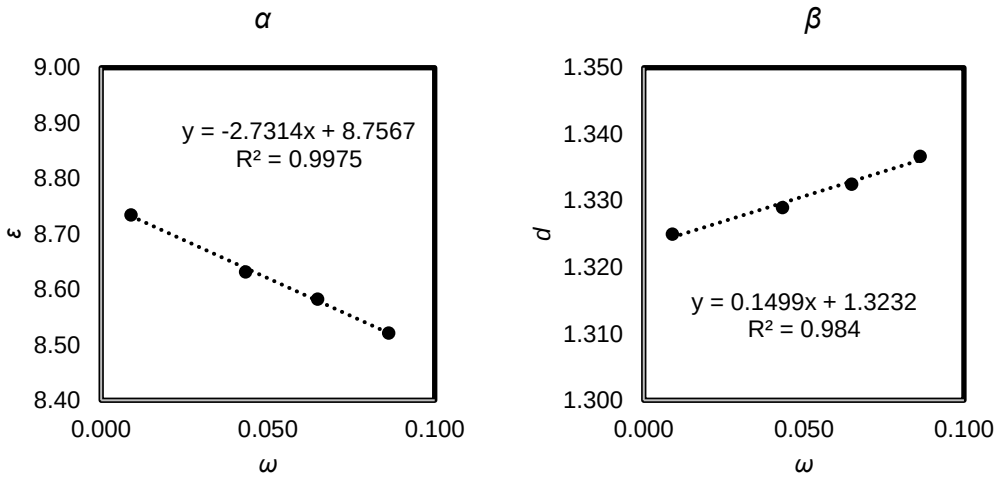

Figure S10. Plot of 7F1AL-POSS solution in dichloromethane. (α); dielectric constant to weight fraction, (β); density to weight fraction.

3. Balls and sticks models

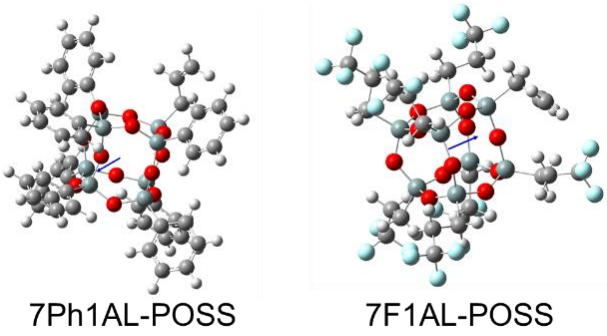

Figure S11. Balls and sticks models of 7Ph1AL-POSS, 7F1AL-POSS structure, optimized in vacuum, calculated from B3LYP 6-31G(d). The direction of the dipole vectors was described using blue arrow as a from their negative to their positive poles.

4. Illustrations of frontier molecular orbitals

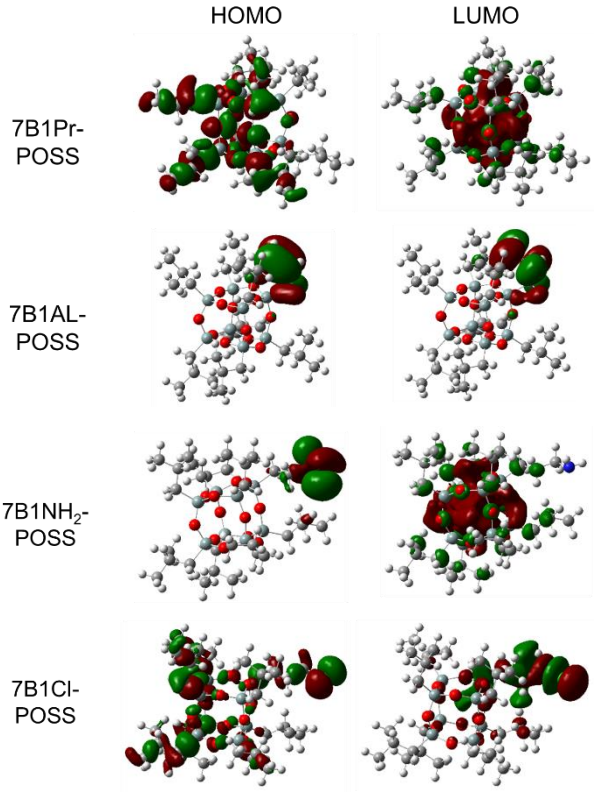

Figure S12. Illustrations of frontier molecular orbitals HOMO and LUMO orbital of substituted POSS calculated B3LYP/6-31G(d) level of theory (isovalue: 0.02). The green lobes represent the negative lobe, and the red lobes represent the positive lobe. The structures are visualized with GaussView 6 software.

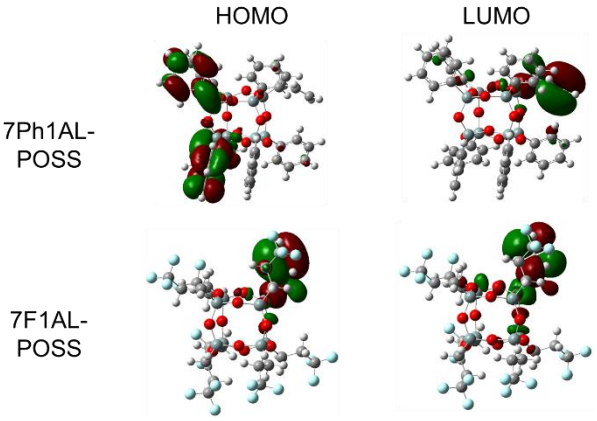

Figure S13. Illustrations of frontier molecular orbitals HOMO and LUMO orbital of substituted POSS calculated B3LYP/6-31G(d) level of theory (isovalue: 0.02). The green lobes represent the negative lobe, and the red lobes represent the positive lobe. The structures are visualized with GaussView 6 software.