Supporting Information

Phase Transition and Molecular Assembly Structure of Ellagic Acid Ester Derivative

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Experimental section

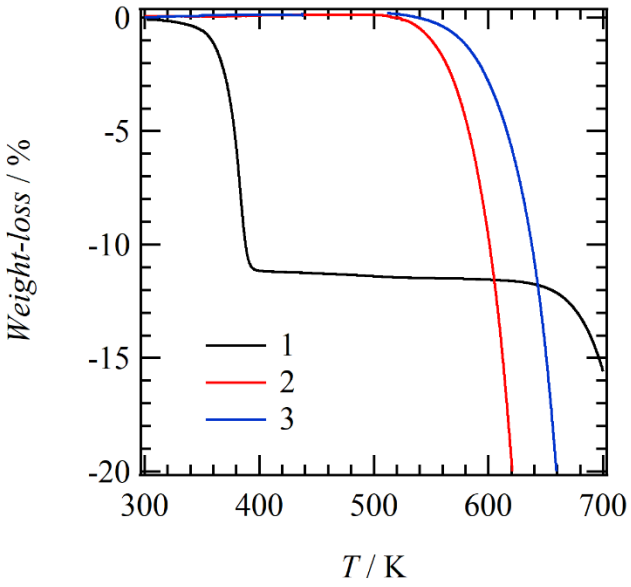

Figure S1. TG diagrams of crystals **1**, **2**, and **3**.

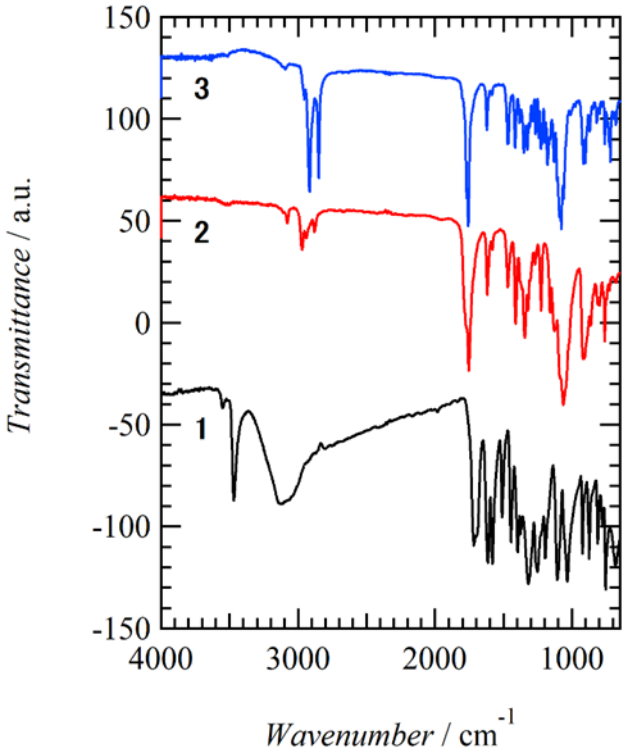

Figure S2. IR charts of crystals **1**, **2**, and **3** at KBr pellets.

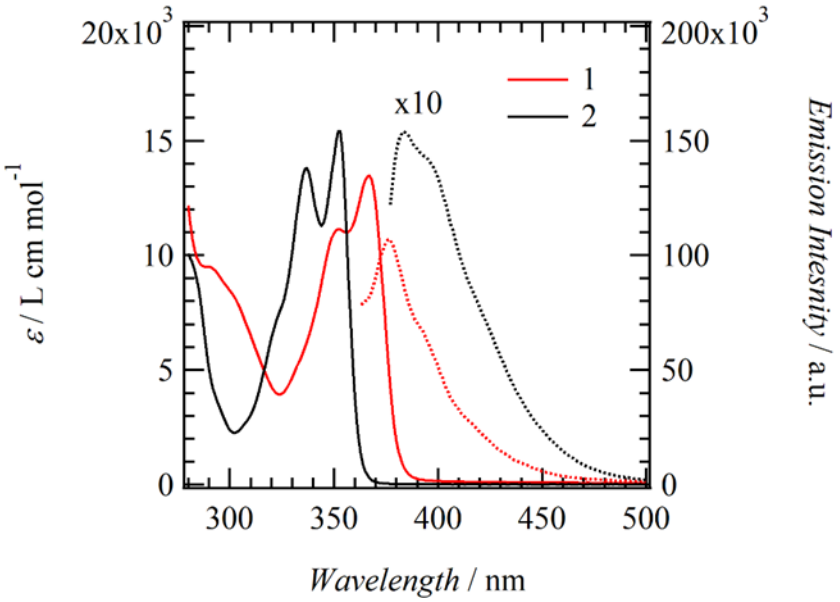

Figure S3. UV (solid line) and fluorescence (dashed line) spectra of **1** and **2** in THF. The emission intensity of **2** was ten times enlarged in contrast with that of **1**.

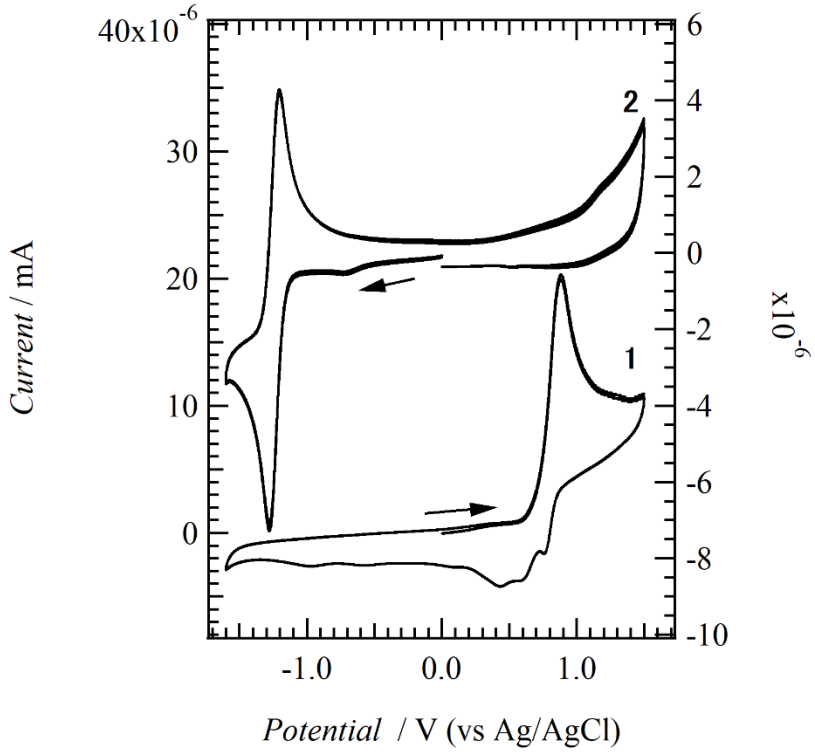

Figure S4. CV charts of **1** and **2** in THF (vs Ag/AgCl 0.1 M $TBABF_4$). The oxidation and reduction waves were observed in **1** and **2**, respectively.

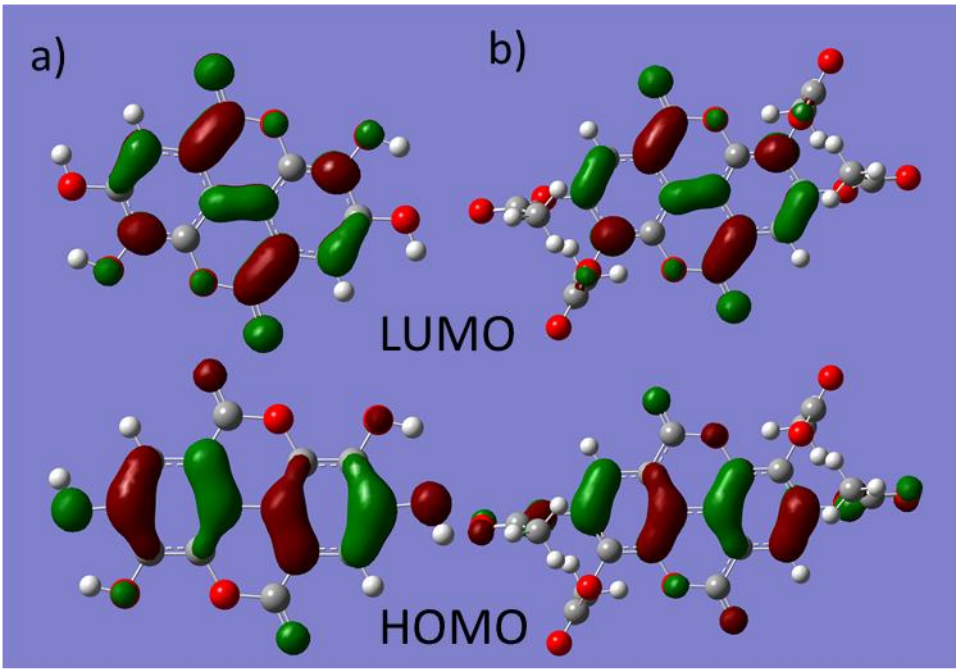

Figure S5. Theoretical DFT calculations of a) HOMO and b) LUMO for **1** (left) and methyl ester derivative (right) based on B3LYP/6-311G+(2d, p) basis set.

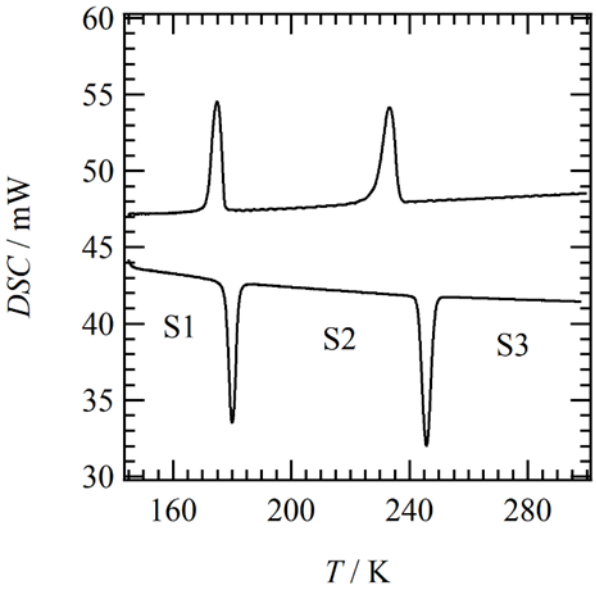

Figure S6. DSC chart of **2** in the temperature range from 150 to 300 K, where three kinds of solid phases of S1, S2, and S3 were reversibly observed.

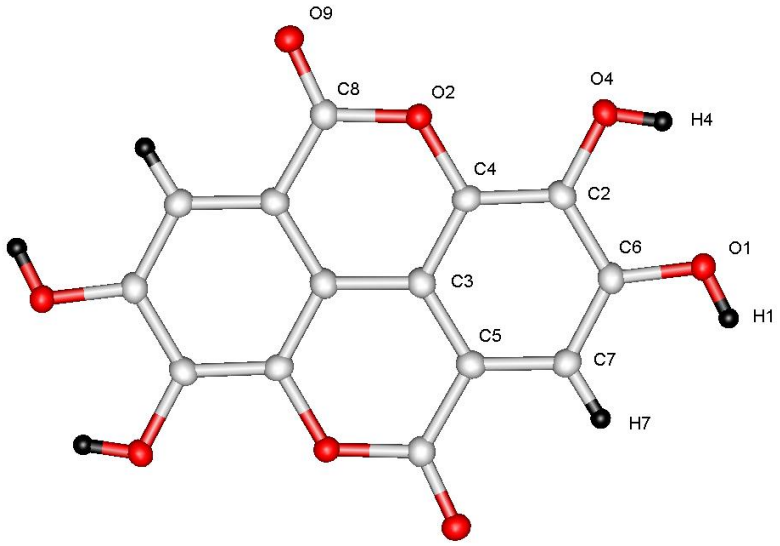

Figure S7. Atomic numbering scheme of molecule **1** in the single crystal X-ray structural analysis.

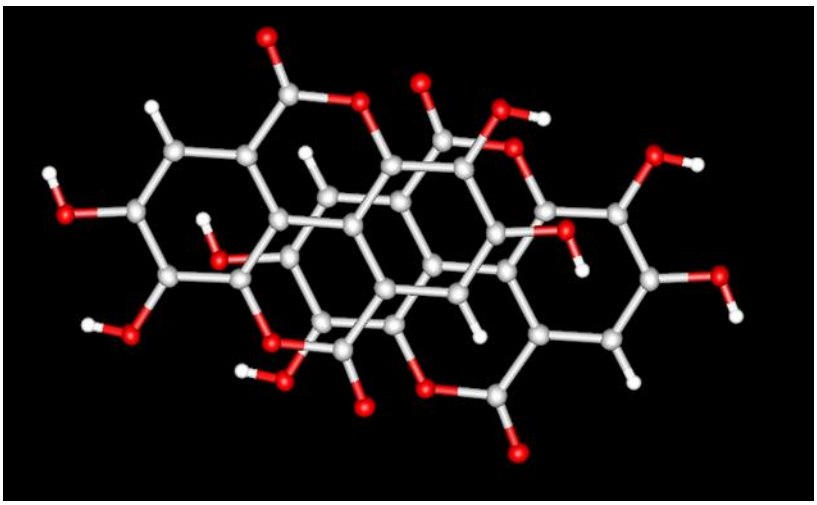

Figure S8. The π-stacking arrangement in the regular stack in **1**.

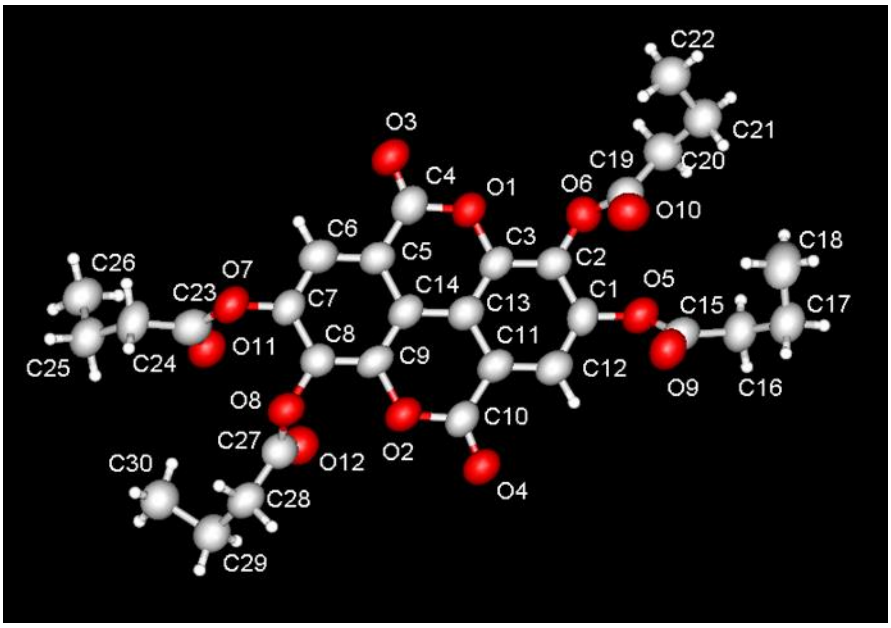

Figure S9. Atomic numbering scheme of molecule **2** in the single crystal X-ray structural analysis.

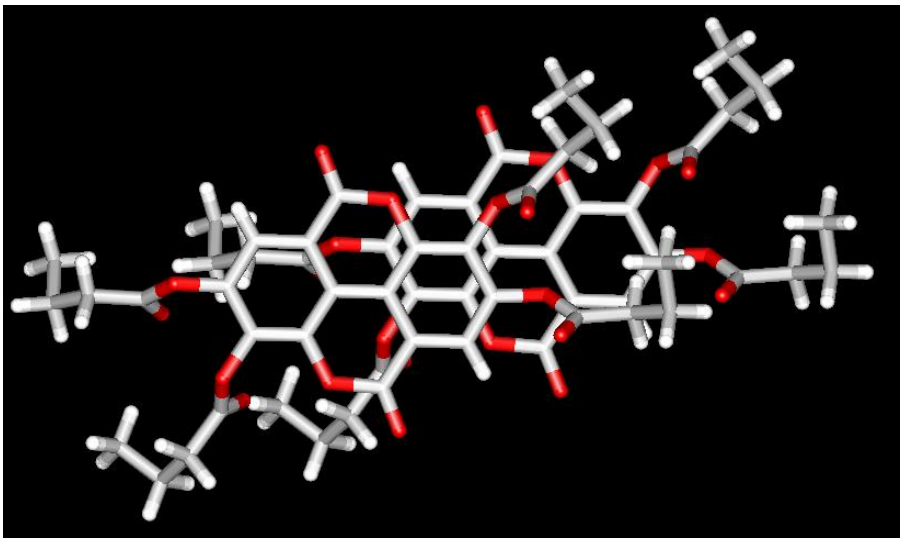

Figure S10. The π-stacking arrangement in the regular stack in **2**.

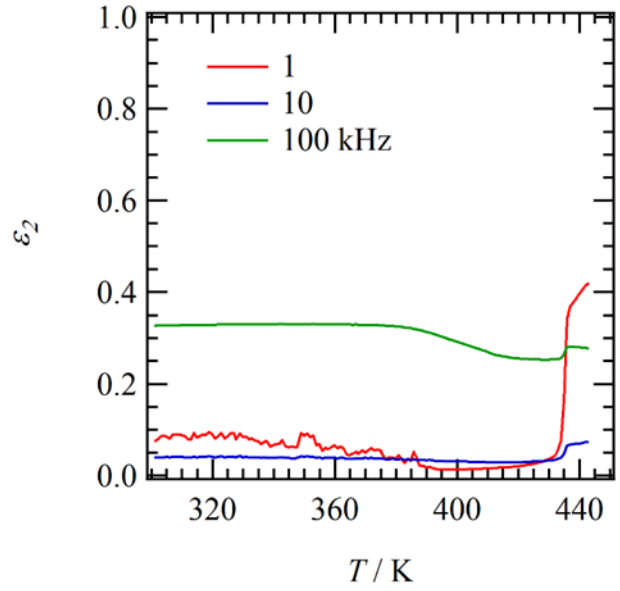

Figure S11. Imaginary part of dielectric constant **3**.

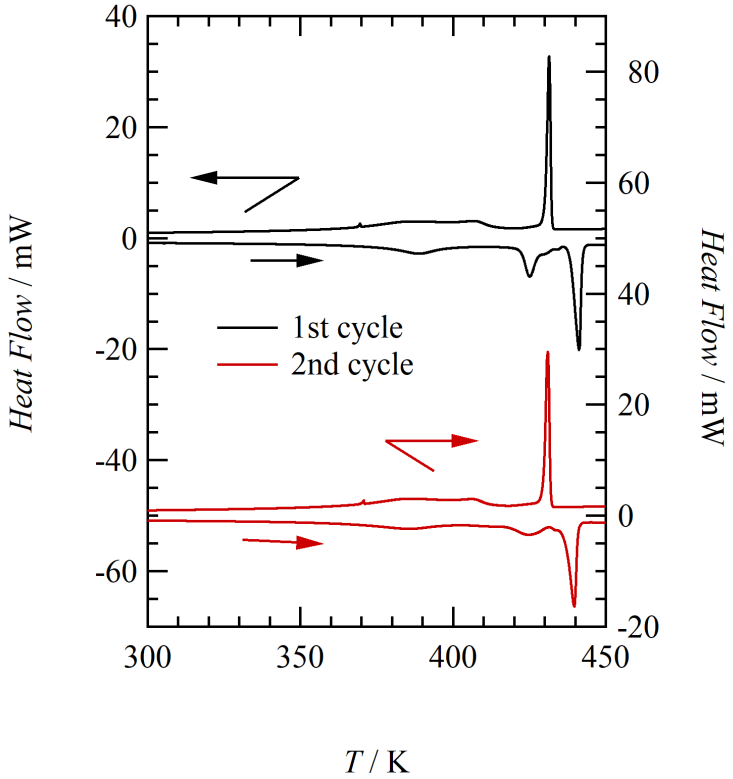

Figure S12. The DSC chart of **3** in the first and second thermal cycle.

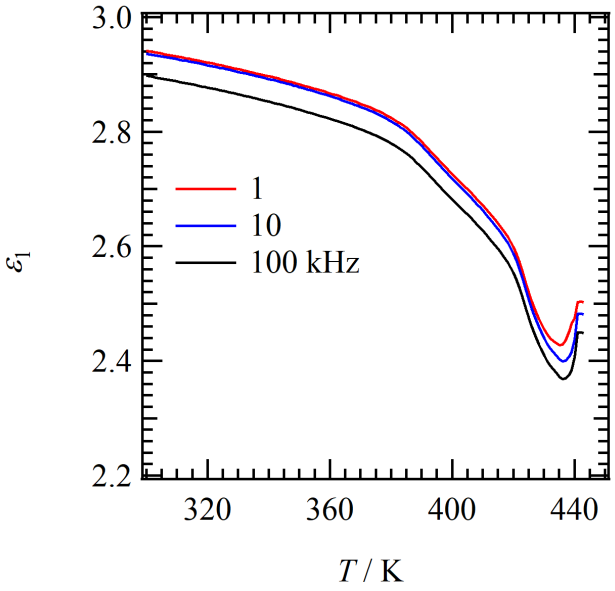

Figure S13. Real part of dielectric constant **3** in the first heating process.