Structural Analyses with Spectroscopic and Computational Studies of Organogels Formed by Liquid-crystalline Phenyl Benzoates

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In our previous works, it has been found that some liquid-crystalline phenyl benzoates with several organic solvents can form physical gels.[1,2] While the correlation between molecular structures and gelation is not elucidated. Meanwhile, it has been reported in our publication[2] that 2-oxochromene-6-yl 4-alkoxybenzoates (Compounds **3**-n, Figure 1) with organic solvents were self-assembled by electrostatic interaction between coumarin skeletons, supporting in UV-Vis and TD-DFT.

In this work, self-assembly phenomena of gelation in organic solvents with phenyl benzoates containing a fluoroalkyl group (Compounds **1**-n and **2**-n, Figure 1) or a coumarin skeleton (Compounds **3**-n) were analyzed by spectroscopic and computational studies.

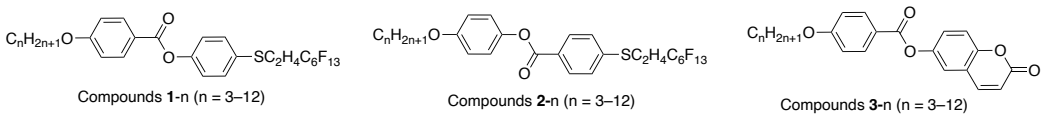

Figure 1. Chemical structures of compounds **1**-n, **2**-n, and **3**-n.

Optimized structures as a dimer for compounds **1**-8 and **2**-8, and each formation enthalpies (ΔH_f) are shown in Figure 2. The gel-sol transition enthalpies for propylene carbonate gels ($\Delta H_{gel\text{-}sol}$) with compounds **1**-8 and **2**-8 at room temperature estimated 36.6 kJ mol^{-1} and 12.5 kJ mol^{-1}, respectively. self-assembly phenomena for gelation with compounds **1**-8 and **2**-8 may be driven by π–π interaction and fluorophilic effect, respectively, since absolute value of $\Delta H_{gel\text{-}sol}$ $\Delta_f H$ are similar values.

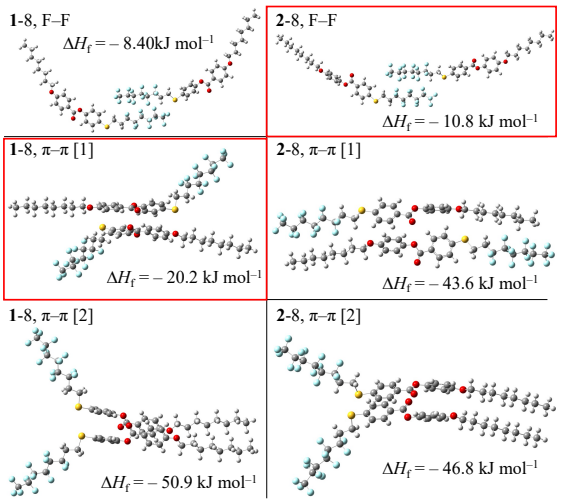

Figure 2. Optimized geometries of compounds **1**-n and **2**-n as a dimer and DFT-calculated formation enthalpy ($\Delta_f H$) using the M06/6-311G (d) level.

In this presentation, effect of polar functional group on gelation, which compared with compounds **1**-n and **3**-n, analyzed by XRD and IR will be reported.

1) B-P. Cao, *et al.*, *J. Fluorine Chem.*, **2019**, *226*, 109348. 2) Y. Endo *et al*, *Chem. Lett*. **2023**, *52*, 337.