# Gel—Sol transition points of Binary Organogels Comprising p-Chlorophenol and AOT: Analyzed by Hansen Solubility Parameters

## Katsura Nishiyama,<sup>1, \*</sup> Kei Ezaki,<sup>1</sup> and Yukiteru Katsumoto<sup>2</sup>

<sup>1</sup>Department of Environmental Technology, Meijo University, Tempaku, Nagoya 468–8502, Japan <sup>2</sup>Department of Chemistry, Fukuoka University, Fukuoka 814–0180, Japan knis@meijo-u.ac.jp\*

#### Abstract

Organogels comprise gelator(s) and solvents where both components have organic nature. *p*-Chlorophenol and a surfactant AOT, bis(2-ethylhexyl)sulfosuccinate serve as organogelators in nonpolar solvents [1, 2], if they are combined in solvent. We have studied such binary organogel structures, optical properties, and mechanical properties or Young's modulus, in our earlier publication [2]. Thermal properties have not been analyzed adequately yet with conventional procedures. In this contribution we show Hansen solubility parameters can be applied to go over gel–sol points of the binary organogel systems. To our knowledge, this study firstly applies Hansen solubility parameters to binary organogels.

#### Materials and data analysis

The reader finds details of organogel synthesis in our previous study [2]. Briefly, equivolume solutions of gelators with a 0.1 mol dm<sup>-3</sup> concentration are mixed to obtain organogels by self-organization. We use a dropping point system DP70, from Mettler Toledo, to get drop points,  $T_{drop}$ , as a measure of the gel–sol transition point. The Hansen solubility parameters package (version 5.0.03) determines the solvent parameters. We use the Hansen distance between materials 1 and 2,  $R_a$ , which is calculated as

$$R_{a}^{2} = 4(\delta D_{1} - \delta D_{2})^{2} + (\delta P_{1} - \delta P_{2})^{2} + (\delta H_{1} - \delta H_{2})^{2}$$
(1)

where *D*, *P*, and *H* stand for dispersion, polarizability, and hydrogen bond terms of solvent interaction, respectively. We take the Hansen distance between the solvent and 3-methylpentance, where the latter corresponds to the effective interaction-site of the gelator AOT.

We study 28 organic solvents in the organogel synthesis. 23 of them are nonpolar solvents and they gel the geletors to form organogel. The remaining systems are with polar solvents, and they stay in sol. Polar solvents are intentionally chosen for comparison.

### Results and discussion

We firstly try to make a clear explanation of  $T_{drop}$  with a help of the boiling points of solvent,  $T_{b, solv}$ . Figure 1 plots  $T_{drop}$  in correlation with  $T_{b, solv}$ . Obviously,  $T_{drop}$  values are scattering around the plot. We see  $T_{b, solv}$  cannot be a suitable measure for  $T_{drop}$  in a global solvent species. With a closer look, meanwhile, we see somewhat positive correlations within four solvent groups (aromatics, acyclic alkanes, cyclic alkanes, cyclic alkenes). We need to have another manner to obtain understandable correlations with  $T_{drop}$ .

In the abscissa of Figure 2, we use  $R_a$  instead. When  $R_a$  goes up,  $T_{drop}$  comes down. Mutual correlation is clearer than plots in Figure 1. The behavior in Figure 2 is reasonable. This is because as the chemical properties are somewhat similar in between the gelator and solvent, the  $R_a$  value becomes small. With more solid interactions between them, we may obtain higher  $T_{drop}$ . At the conference site we talk about more molecular views regarding gelator—solvent interactions.

#### EMLG2022



Figure 1. Plots of  $T_{drop}$  versus  $T_{b, solv}$ . Solvent groups are found inside the graph. Two solvents that are independent of the solvent groups are perhaloalkane, or carbon tetrachloride (|><|), and acyclic alkene, or 2-butyl-1-butene (+). The solid lines are guide to eye.



Figure 2. Plots of  $T_{drop}$  versus  $R_a$ . Solvent groups are found inside the graph. Two solvents that are independent of the solvent groups are perhaloalkane, or carbon tetrachloride (|><|), and acyclic alkene, or 2-butyl-1-butene (+). The solid line is guide to eye.

KN thanks MEXT KAKENHI (16K05750), Japan, for financial help.

#### REFERENCES

- B.A. Simmons, C.E. Taylor, F.A. Landis, V.T. John, G.L. McPherson, D.K. Schwartz, R. Moore, J. Am. Chem. Soc. 123 (2001) 2414–2421.
- [2] S. Katsube, M. Kinoshita, K. Amano, T. Sato, Y. Katsumoto, T. Umecky, T. Takamuku, T. Kaji, M. Hiramoto, Y. Tsurunaga, K. Nishiyama, Langmuir 32 (2016) 4352–4360.