

Relationship between Liquid Crystal and Organogel Formed by Low Molecular Weight Gelators with Coumarin Skeleton

(¹Faculty of Engineering, Yamaguchi University, ²Advanced Technology Institute, Yamaguchi University, ³Graduate School of Sciences and Technology for Innovation, Yamaguchi University) ○ Yuri Hatsuda,¹ Ryo Narusaka,¹ Yuki Morita,² Kosuke Kawabe,³ Hiroaki Okamoto.³

Keywords: Coumarin Skeleton; Organogel; Low Molecular Weight Gelators; Liquid Crystal;

In our previous works¹⁾, it was found that some low molecular weight compounds having liquid crystallinity gelled various organic solvents when compounds were heated and dissolved in solvents and cooled. Gelation was involved in the statement which thermotropic liquid crystal phase were existed. However, the relationship between liquid crystal and gel was not elucidated.

In this study, compounds **1-n** (Fig. 1) were synthesized and examined gelation ability in several organic solvent. Furthermore, it was predicted that molecular arrangements by small angle X-ray diffraction so that the relationship between liquid crystal and gel was considered.

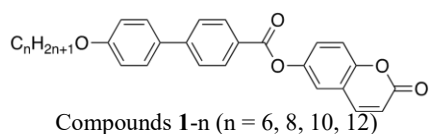


Fig. 1 Chemical structures of compounds **1-n**

Compounds **1-n** added in amount of 2wt% or less were able to gelate 1-octanol, DMSO and PC (Table 1). In PC gel, gelation was possible with a smaller amount of addition by elongation of the alkyl chain in compounds **1-n**.

Table 1 Critical gel concentration in each solvent

Solvents	Compounds (Concentration / wt%)			
	1-6	1-8	1-10	1-12
1-Octanol	G (2.0)	G (0.3)	G (0.8)	G (0.8)
DMSO	G (2.0)	G (1.0)	G (0.6)	G (0.8)
PC	G (2.0)	G (0.8)	G (0.5)	G (0.5)

G = Gel, I = Insoluble, S = Sol

DMSO = Dimethyl sulfoxide, PC = Propylene carbonate

In addition, the peak of X-ray profile was at $2\theta = 2.28^\circ$ (Fig. 2). Molecular modeling of 10wt% PC gel was predicted from the layer spacing (38.7Å) calculated by Bragg's equation. It was predicted that compound **1-10** in PC gel formed fibrous aggregation (Fig. 3).

In this presentation, the relationship of self-assembly structure between the liquid crystal phase of compounds **1-n** and organogels formed by them will be considered.

Ref: 1) F. Zhang *et al.*, *Chem Lett.* **2005**, 34, 8

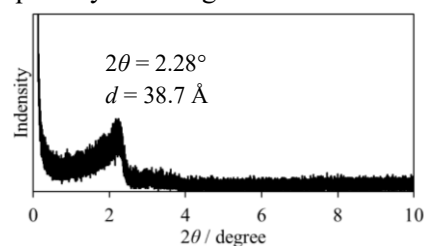


Fig. 2 X-ray profile of 10wt% PC gel formed by compound **1-10**

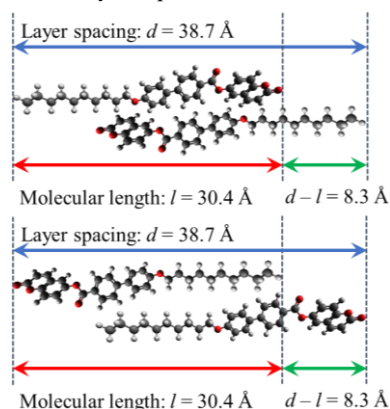


Fig. 3 Prediction of molecular modeling in 10wt% PC gel formed by compound **1-10**