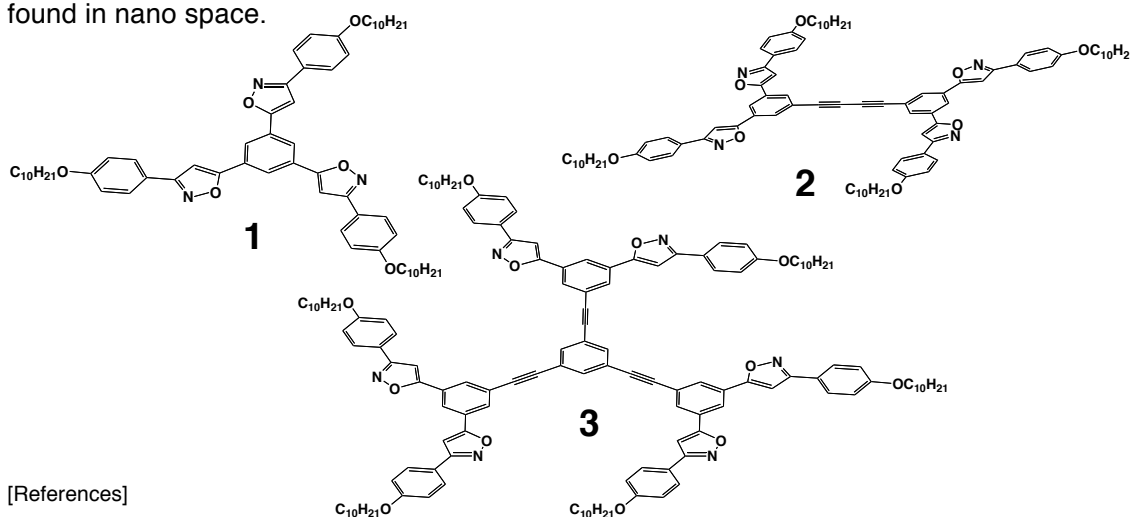


Self-assembly of extended π -conjugated molecules based on phenylisoxazoles

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1,3,5-Tris(phenylisoxazolyl)benzene **1** stacks via π - π stacking interaction to form the supramolecular assemblies. During the studies, we have found that the isoxazole unit is responsible for the intermolecular dipole-dipole interactions to facilitate the self-assembly. When four or six isoxazole units are introduced on a benzene core, the self-assembly should be promoted (**2** and **3**). Their assembling behaviors were studied using ^1H NMR. The association constants were determined by non-linear least square curve fitting analysis (K_a : 3.7 ± 0.3 , 15 ± 1 and $740 \pm 70 \text{ L mol}^{-1}$ for **1** , **2** and **3**). The introduction of the additional three isoxazole units developed the surprising stability for the assembly of **3**. The results suggest that the extended π -conjugated surfaces with the additional isoxazole rings play an important role for the self-assemblies of the phenylisoxazolylbenzene derivatives.

The morphologies of their xerogels were observed by using the field emission scanning electron and atomic force microscopies. The three-dimensional entangled networks were found in nano space.



[References]

- [1] Tanaka, M.; Ikeda, T.; Mack, J.; Kobayashi, N.; Haino, T. *J. Org. Chem* 2011, 76, 5082–5091.
- [2] Haino, T.; Saito, H. *Aust. J. Chem.* 2010, 63, 640-645.
- [3] Haino, T.; Saito, H. *Synth. Met.* 2009, 159, 821-826.
- [4] Haino, T.; Tanaka, M.; Fukazawa, Y. *Chem. Commun.* 2008, 468-470.