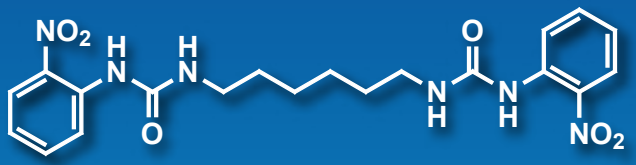
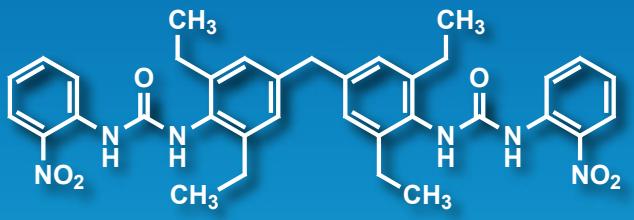
Steed's Supramolecular Gelators for Pharmaceutical Crystallization and Polymorph Control



1,1'-(Hexane-1,6-diyl)bis[3-(2-nitrophenyl)urea]
1g / 5g
[H1655]



1,1'-[Methylenebis(2,6-diethyl-4,1-phenylene)]-bis[3-(2-nitrophenyl)urea
1g / 5g
[M3072]

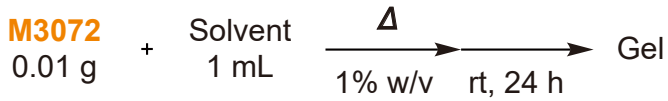
Advantages

- **H1655** can form gels at 1% weight to volume
- Applicable to acetonitrile, methanol, ethanol and acetone

- **M3072** can form robust, stable, and translucent gels
- Applicable to acetonitrile, methanol, acetone, ethyl acetate
- Critical gelation concentration : <1% w/v

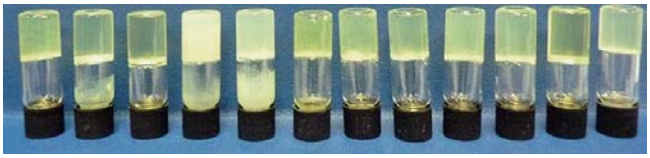
Application

Gel Preparation



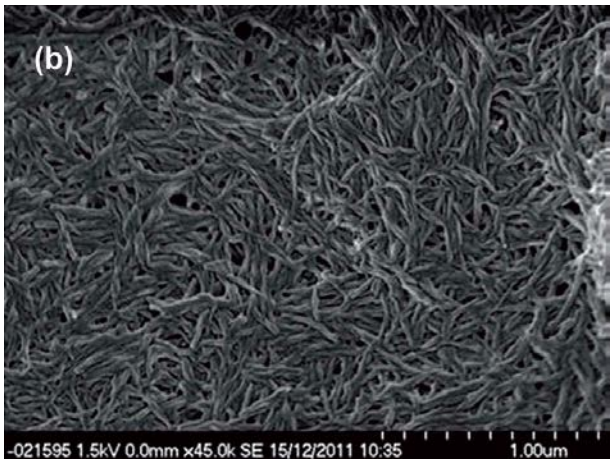
M3072 (0.01 g) is heated in 1 mL of solvent (1% w/v) in a sealed vial until fully dissolved and then cooled to room temperature. After 24 h, gel formation is characterised by a simple vial inversion test; if the solvent is fully immobilised it is considered to have gelled.

(a)



(a) Organogels formed by **M3072** in (left to right) dichloromethane, chlorobenzene, 1,2-dichlorobenzene, benzene, toluene, acetonitrile, methanol, ethanol, 1-propanol, 1-butanol, nitrobenzene and ethyl acetate.

(b) SEM micrograph of the toluene xerogel of **M3072** at 1% w/v.



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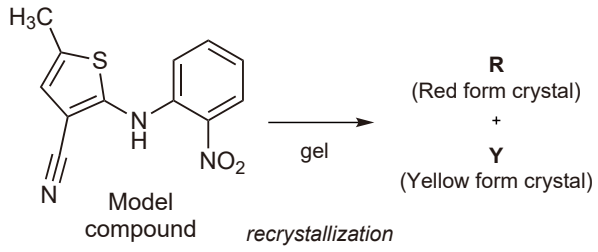
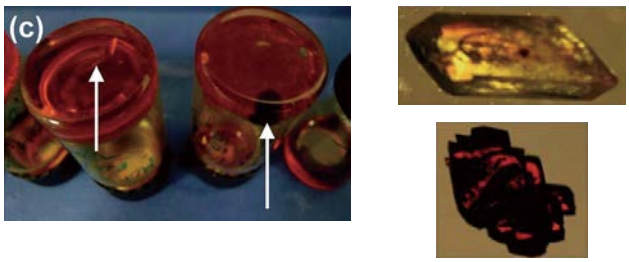
Polymorph Control



1 mL toluene is added to gelator (10 mg) and model compound (100 mg) sealed and heated to 140°C until all solids have dissolved and then immediately placed in an oven at 120°C. The solutions are cooled to 50°C over 23 h and then to rt over a further 10 h. Crystallization generally takes place over several hours to weeks.



(c) **Y**-form crystals growing in a toluene gel of non-specific gelator on the left and **R**-form crystals growing in toluene gel of model compound, (right; arrows point to individual crystals). Isolated gel-grown crystals of the **Y** and **R** forms.

Reference J. A. Foster, K. K. Damodaran, A. Maurin, G. M. Day, H. P. G. Thompson, G. J. Cameron, J. C. Bernal, J. W. Steed, *Chem. Sci.* **2017**, *8*, 78. https://doi.org/10.1039/C6SC04126D

Introduction to the Researcher

Professor **Jonathan W. Steed, Ph. D.**
Durham University

The Steed Research Group

Supramolecular Chemistry, Molecular Sensors, Supramolecular Gels, and Crystallography and Solid Form

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Tel : 800-988-0390 / 021-67121386
Fax : 021-6712-1385
E-mail : Sales-CN@TCIchemicals.com

TOKYO CHEMICAL INDUSTRY CO., LTD.
Tel : +81 (0)3-5640-8878
E-mail : globalbusiness@TCIchemicals.com