

Dicyclohexylammonium bromoacetate: a low molecular weight gelator with one-dimensional SAM synthon

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Supplementary material

Table S1 Monocarboxylic acids with SAM synthon proven to form gels.

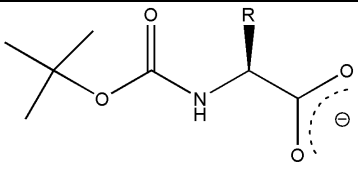
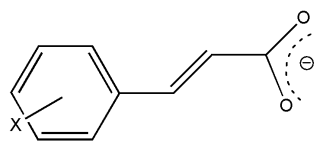
Entry	Carboxylic acid	R/X	Synthon	Database refcode	Source
1.		R = H	1D	FAYNIE	Sahoo <i>et al.</i> , 2012
		X = 4-Br	1D	JAMWOK	Trivedi <i>et al.</i> , 2004
		X = 4-Me	1D	JAMWUQ	
		X = H	1D	JAMXAX	
		X = 4-Cl	1D	JAMWIE	
2.					Trivedi <i>et al.</i> , 2004 Trivedi <i>et al.</i> , 2003
		X = 4-NO ₂	1D	RATZES	Trivedi <i>et al.</i> , 2005

Table S2 Gelation properties of (**I**).

In a typical experiment dicyclohexylammonium bromoacetate (40 mg) was dissolved in appropriate organic solvent (0.5 ml) by heating. Then, the clear solution was left in test tube unperturbed to cool to room temperature. To examine formation and quality of gel, test tube was inverted by 180°. The system was regarded as a true organogel if the contents of the test tube did not flow (Fig S5). The gel prepared in test tube was then heated in an oil bath. T_{gel} temperature was noted when a whole sample become a sol.

Entry	Solvent	MGC ^a [wt %] ^b	T_{gel} ^c
1.	CCl ₄	S	
2.	Chloroform	S	
3.	Cyclohexane	IS	
4.	<i>n</i> -hexane	IS	
5.	Toluene	WP	
6.	Chlorobenzene	S	
7.	<i>o</i> -xylene	WP	
8.	Xylenes	WP	
9.	DMF	8.00	133
10.	Ethyl acetate	S	
11.	DMSO	8.00	96
12.	1,4-dioxane	S	
13.	THF	S	
14.	2-methoxyethanol	S	
15.	Methylmethacrylate	S	

^aMGC = minimum gelator concentration at room temperature. ^bwt % = g per 100 ml of solvent. ^c T_{gel} = gel-to-sol dissociation temperature in °C; S = solution, IS = insoluble, WP = white precipitate

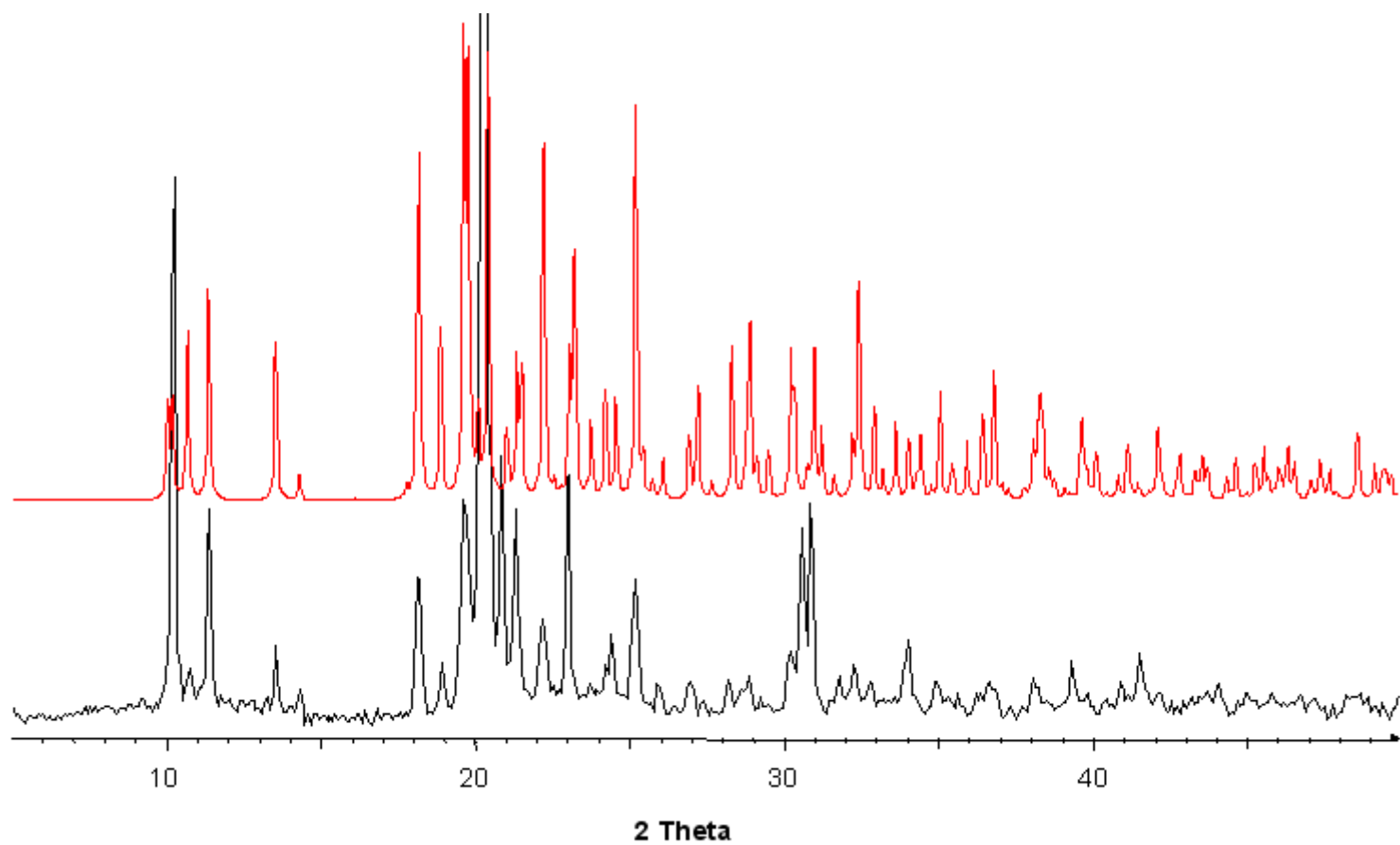


Figure S1 Experimental X-ray powder pattern (black, $T = 298\text{ K}$, $\text{Cu-K}\alpha_1$) and simulated powder pattern (red, $T = 100\text{ K}$, $\text{Mo-K}\alpha$) based on the results from single-crystal X-ray diffraction for the title salt.

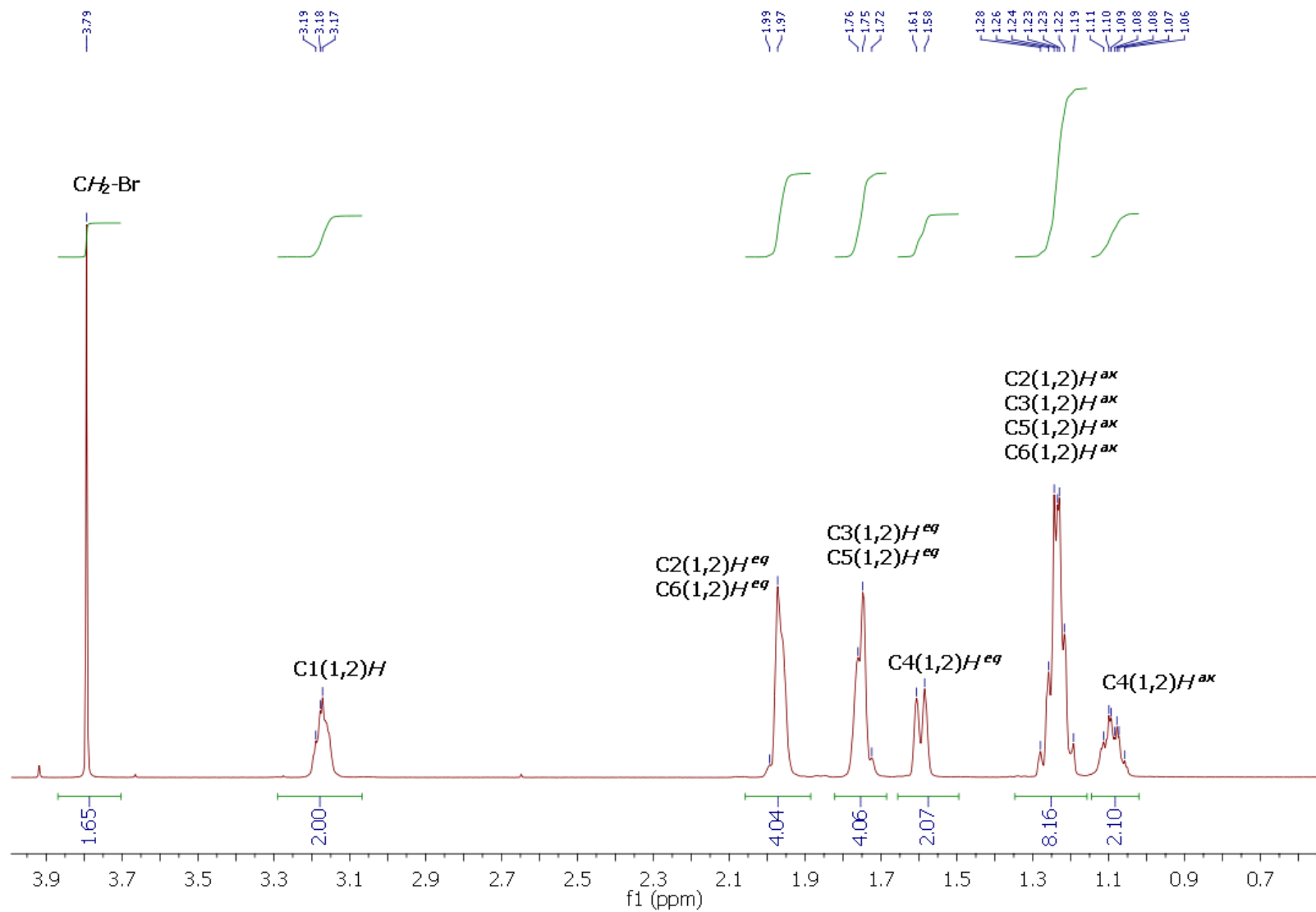


Figure S2 NMR spectrum of the title salt (**I**).

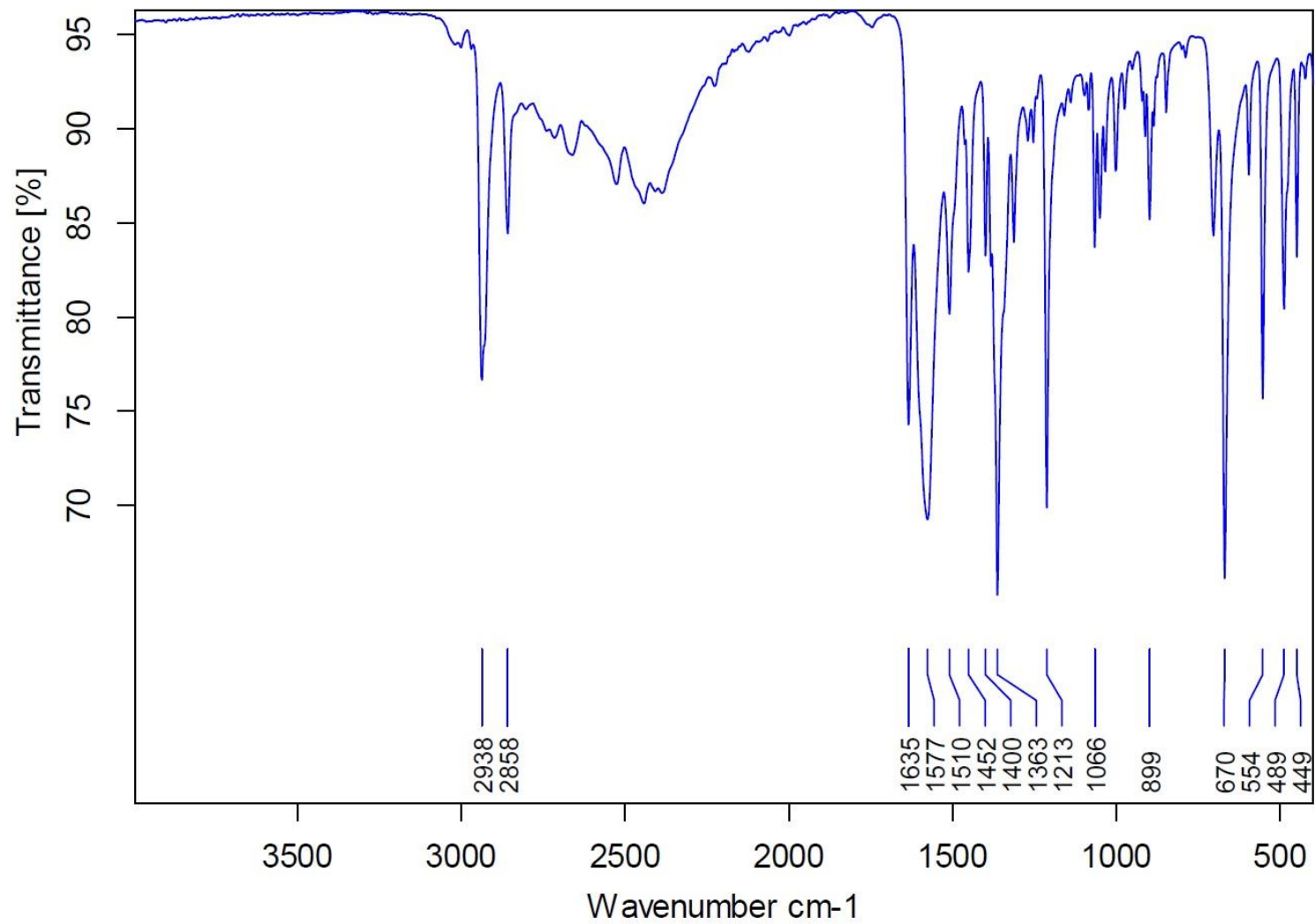


Figure S3 IR spectrum of the title salt (**I**).

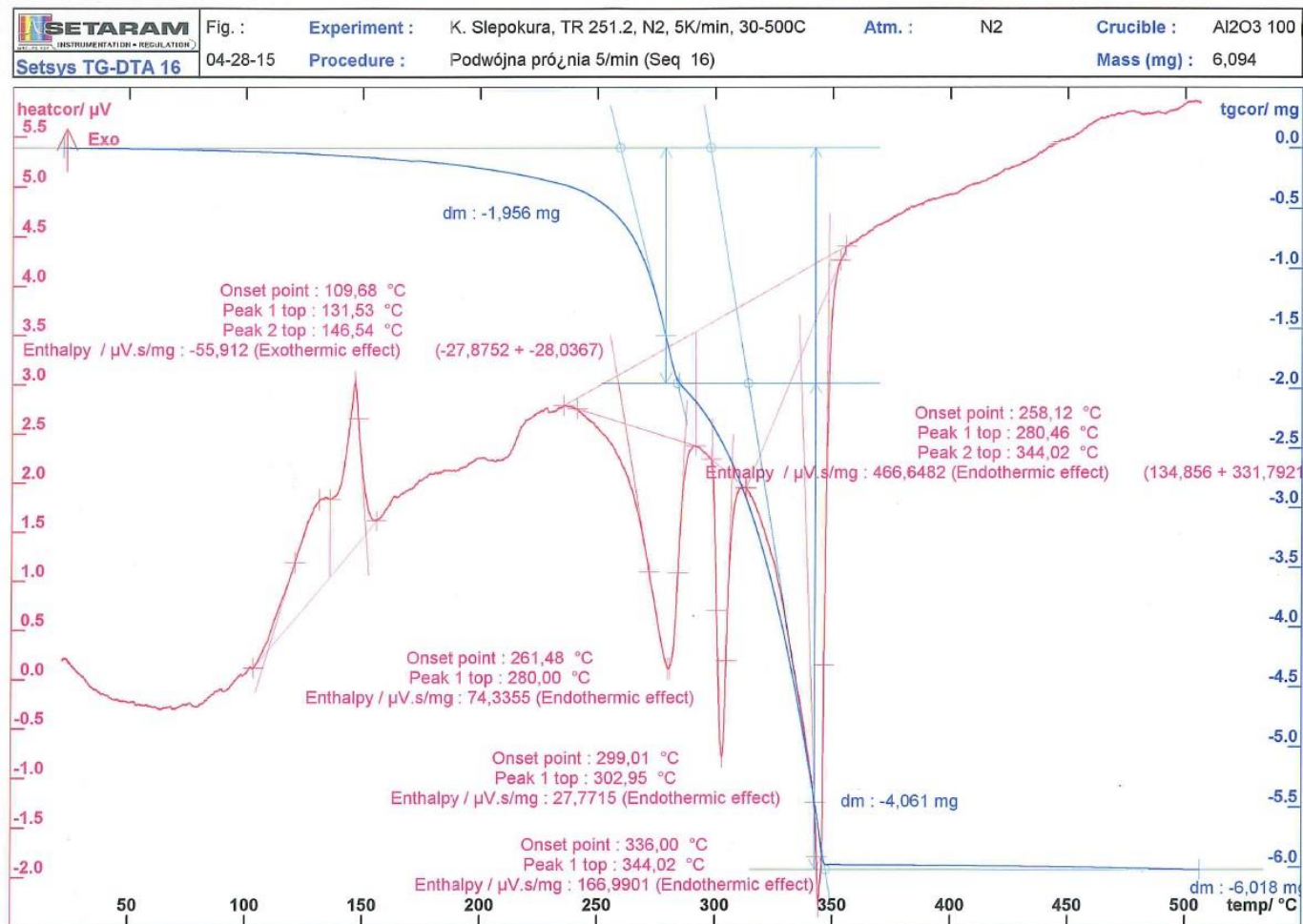


Figure S4 TG-DTA plot for the title salt (I).

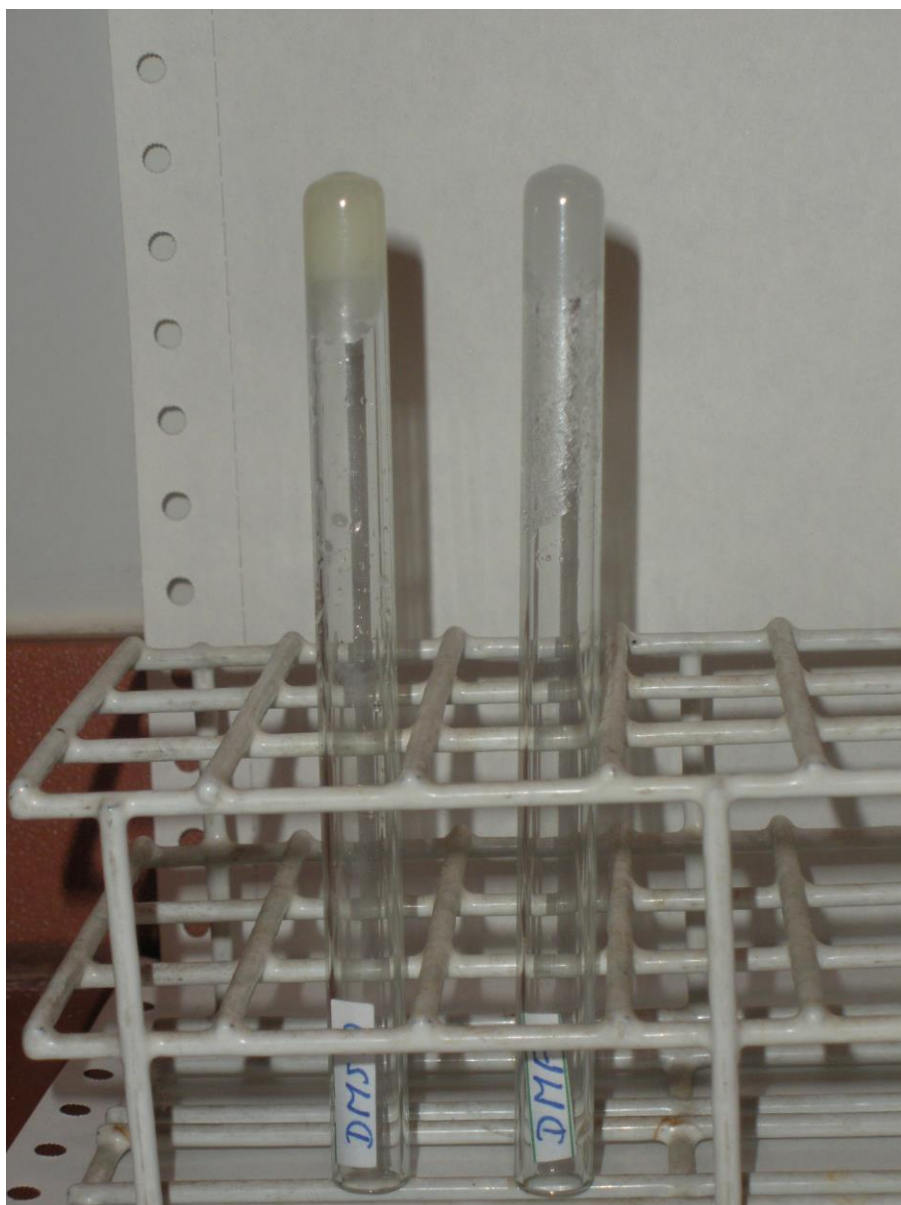


Figure S5 Photographs of the organogels: left (**I**) in DMSO and right (**I**) in DMF. Test tube diameter: 8 mm.