

Supporting Information

Tuning morphology and properties of cellulose-based aerogels and xerogels by the introduction of tosyl moieties

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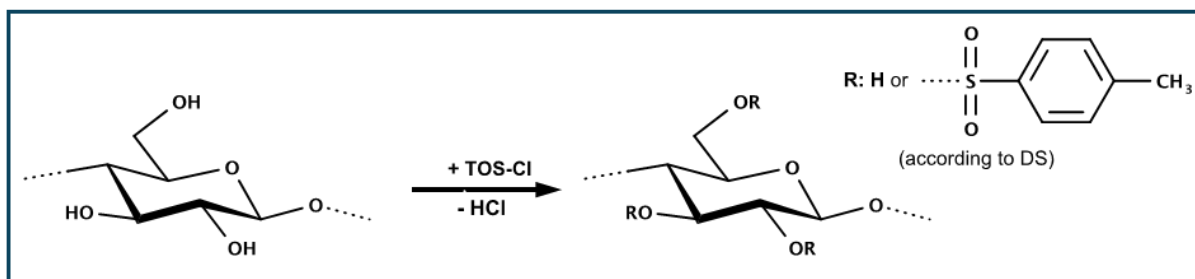


Figure S1. Reaction scheme for the synthesis of tosyl cellulose

Table S1. Conditions for and results of the synthesis of tosyl cellulose (TOSC) by conversion of by homogeneous conversion of microcrystalline cellulose (MCC) in *N,N*-dimethylacetamide with tosylchloride (TOS-Cl) in the presence of triethylamine (Et₃N). DS_{tosyl} and DS_{Cl} are degree of tosylation and chlorination respectively.

Sample	Molar equivalents ^a			Results	
	LiCl	Et ₃ N	TOS-Cl	DS _{tosyl} ^b	DS _{Cl} ^b
MCC	-	-	-	-	-
TOSC 0.22	7.0	1	0.5	0.22	0.02
TOSC 0.56	7.0	2	1.0	0.56	0.04
TOSC 1.26	7.0	3	1.5	1.26	0.07

^amol per mol anhydroglucose units; ^b degrees of substitution with tosyl groups (DS_{tosyl}) and deoxy-chloro groups (DS_{Cl}).

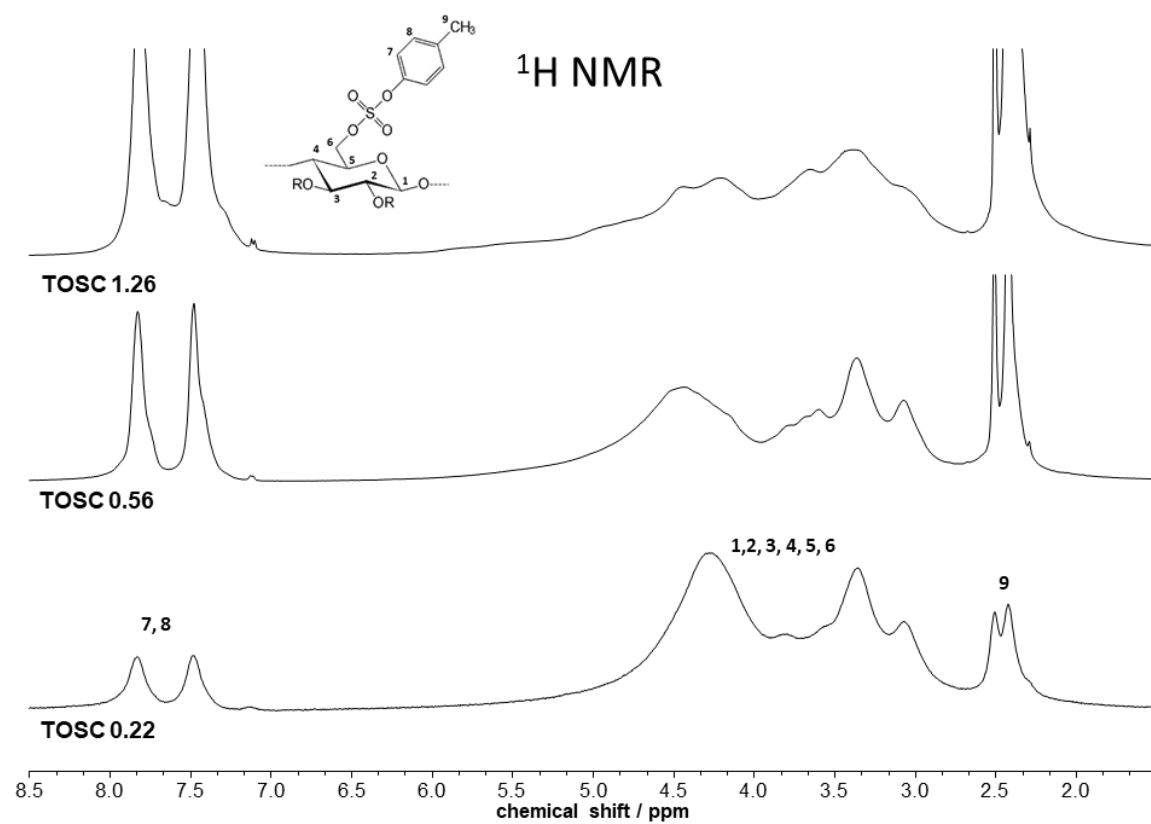


Figure S2. ^1H -NMR spectra of tosyl cellulose of different degrees of substitution.

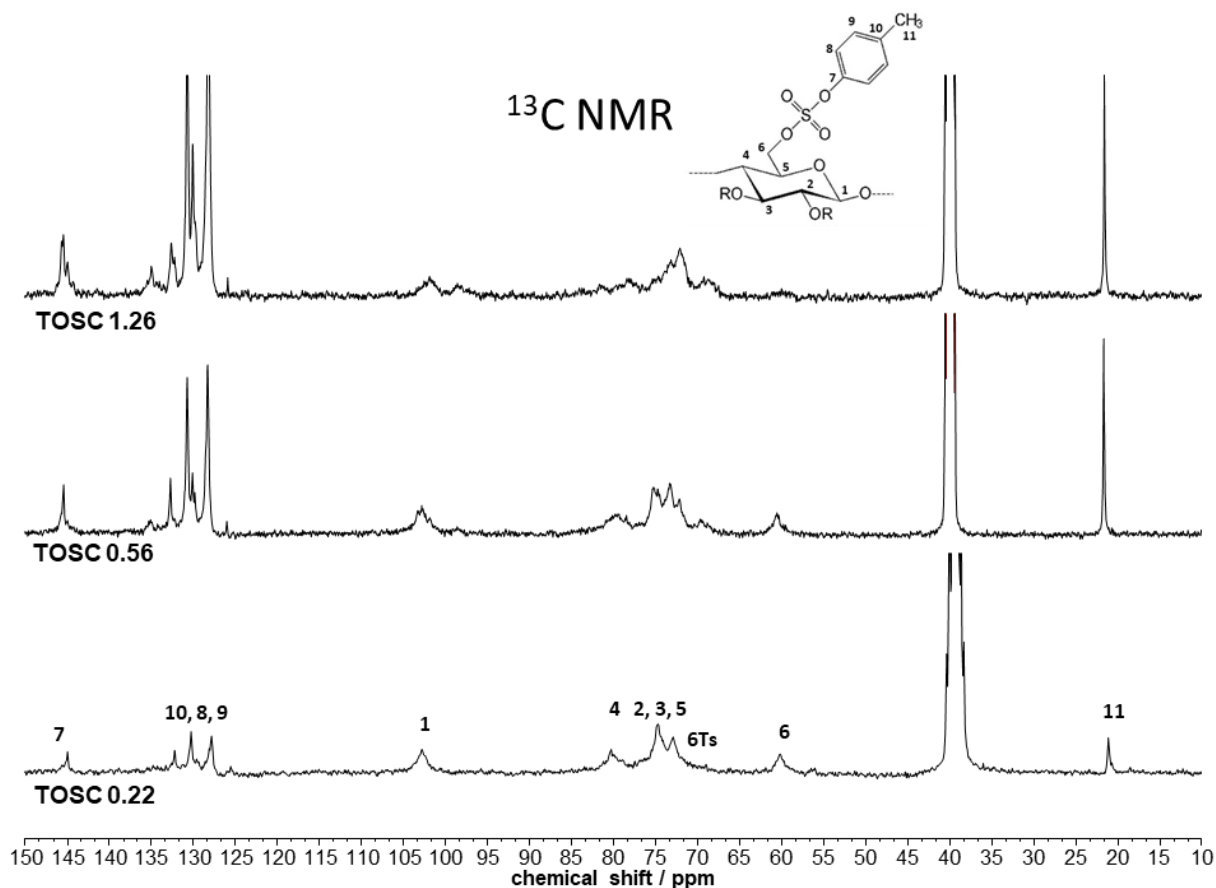


Figure S3. ¹³C-NMR spectra of tosyl cellulose of different degrees of substitution.

The degrees of substitution (DS) were calculated based on the following formula:

$$DS_{Tosyl} = \frac{\left(\frac{S\%}{100\%}\right) \cdot M_{AGU} \cdot M_{Cl}}{M_S \cdot M_{Cl} - \left(\frac{S\%}{100\%}\right) \cdot M_{Cl} \cdot (M_{Tosyl} - M_H) - \left(\frac{Cl\%}{100\%}\right) \cdot M_S \cdot (M_{Cl} - M_H - M_O)} \quad (S1)$$

$$DS_{Cl} = \frac{\frac{Cl\%}{100\%} \cdot (M_{AGU} + (M_{Tosyl} - M_H) \cdot DS_{Tosyl})}{M_{Cl} \cdot (M_{Cl} - M_H - M_O) - \frac{Cl\%}{100\%}} \quad (S2)$$

where S%, Cl% are the percent of sulfur or chlorine found by elemental analysis. M_{AGU} , M_{Tosyl} , M_{Cl} , M_S , M_O and M_H are the molar mass of the anhydroglucose repeating unit, the tosyl group, chlorine, sulfur, oxygen and hydrogen, respectively.

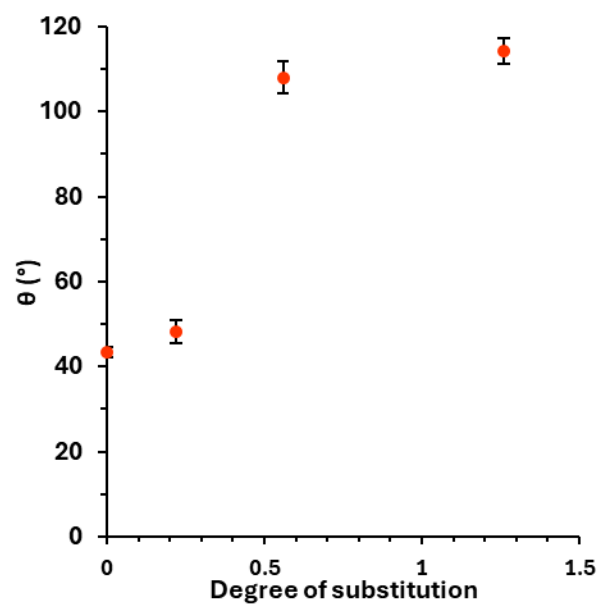


Figure S5.

Contact angle for films made from MCC and TOSC of different DS, coagulated in ethanol and dried from ethanol, as a function of the degree of substitution.