Tosylcellulose synthesis in aqueous medium

Pierre-Henri Elchinger,^{a,b} Pierre-Antoine Faugeras,^{a,b} Chouki Zerrouki,^c Daniel Montplaisir,^b François Brouillette^b and Rachida Zerrouki^{*a}

Complementary Data:

NMR Data of compound with DS: 0.97 (entry 7 table 1).

P8 dans DMSO-d6/LiCl - Spectre RMN 1H Service de RMN - Universite de Limoges



P8 dans DMSO-d6/LiCl - Spectre RMN 1H Service de RMN - Universite de Limoges



XPS Data of the same compound with a DS of: 0.96 (entry 7 table 1).

First measure point:

Surva/2 Lens Mode:Hybrid Resolution:Pass energy 160 Anode:Mono(A1 (Mono))(225 W) Step(meV): 1000.0 Dwe11(ms): 100 Sweeps: 1 Acquisition Time(s): 130 Acquired On :12/03/01 10:07:53 C/N :On



Second measure point:

Survb/4 Lens Mode:Hybrid Resolution:Pass energy 160 Anode:Mono(A1 (Mono))(225 W) Step(meV): 1000.0 Dwel1(ms): 100 Sweeps: 1 Acquisition Time(s): 130 Acquired On :12/03/01 10:12:19 C/N :On



Third measure point:

Survc/6 Lens Mode:Hybrid Resolution:Pass energy 160 Anode:Mono(A1 (Mono))(225 W) Step(meV): 1000.0 Dwel1(ms): 100 Sweeps: 1 Acquisition Time(s): 130 Acquired On :12/03/01 10:16:47 C/N :On



DRX measurements Information:

Example of DRX spectra deconvolution:



Data: Data1_A Model: Gauss			
Chi^2/	Chi^2/DoF = 0.23634		
R^2	R^2 = 0.99084		
y0	4.23257	± 1.08907	
xc1	22.70216	± 0.02527	
w1	1.72661	± 0.25165	
A1	24.71418	± 18.8747	
xc2	21.28608	± 1.06636	
w2	2.82333	± 1.29396	
A2	27.06676	± 27.24676	

Debye-Scherrer equation :

 $L_{hkl} = \frac{K \times \lambda}{\Delta \theta \times \cos(\theta)}$

 L_{hkl} is the crystallite size in the direction perpendicular to plane with hkl as Miller index. λ is the X-ray wavelength. $\Delta \theta$ is the half-width of the diffraction peak. Estimation of degree of crystallinity:

$$CI = \frac{I_{002} - I_{am}}{I_{002}} \times 100 \qquad \text{Or} \qquad CI = \frac{A_{002}}{A_{002} + A_{am}} \times 100 \quad (I \text{ and } A \text{ are the intensity and the area of the diffraction peak})$$