

Alkali induced changes in spatial distribution of functional groups in carboxymethylated cellulose

Cellulose

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Table S1 Results of carboxyl group content, methylene blue sorption and FTIR ratio measurements on fibers from the additional set of treatments in reaction media containing 4 mol/L NaOH with the ηp sequence. Mean values from three replicates are shown along with their standard deviation (in parentheses)

Treatment variables		Carboxyl group content (mmol/kg)		MB Sorption (mmol/kg) ^c	Normalized FTIR absorbance ^d	
MCA (mol/L)	Temp. (°C)	A-B ^a	Cond. ^b		ATR	KBR
0.161	30	192.5 (0.8)	— ^e	40.2 (1.3)	0.349 (0.049)	0.297 (0.034)
	50	168.9 (4.1)	—	35.2 (0.2)	0.290 (0.006)	0.237 (0.009)
0.322	30	317.7 (2.9)	284.9 (5.5)	64.0 (3.0)	0.564 (0.005)	0.338 (0.023)
	50	285.2 (1.1)	269.0 (11.9)	60.1 (1.4)	0.534 (0.025)	0.315 (0.031)

^a back titration, ^b conductometric titration, ^c methylene blue sorption, ^d absorbance intensities at 1591 cm⁻¹ (ATR) and 1600 cm⁻¹ (KBr, i.e. transmittance) normalized with respect to the absorbance intensity at 1156 cm⁻¹, ^e signifies not measured.

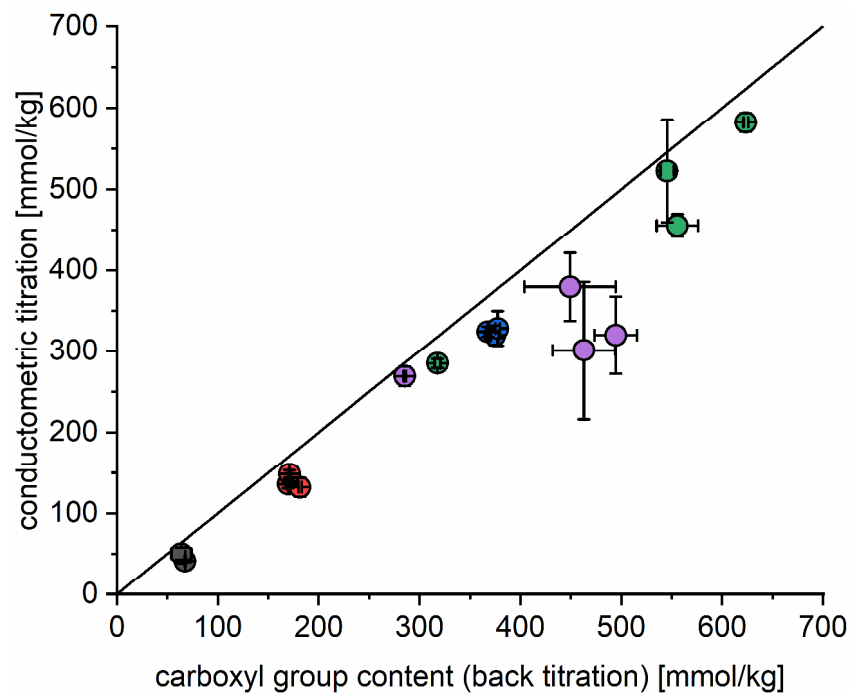


Fig. S1 Comparison of carboxyl contents determined with conductometric titration vs. back titration, including data from the additional treatments. The diagonal line in each plot represents a 1:1 relationship between the abscissa and ordinate. The marker colors represent treatment sets: demineralized and no-MCA blank (●), in 0.5 mol/L NaOH at 30°C (●), in 0.5 mol/L NaOH at 50°C (●), in 4 mol/L NaOH at 30°C (●) and in 4 mol/L NaOH at 50°C (●)

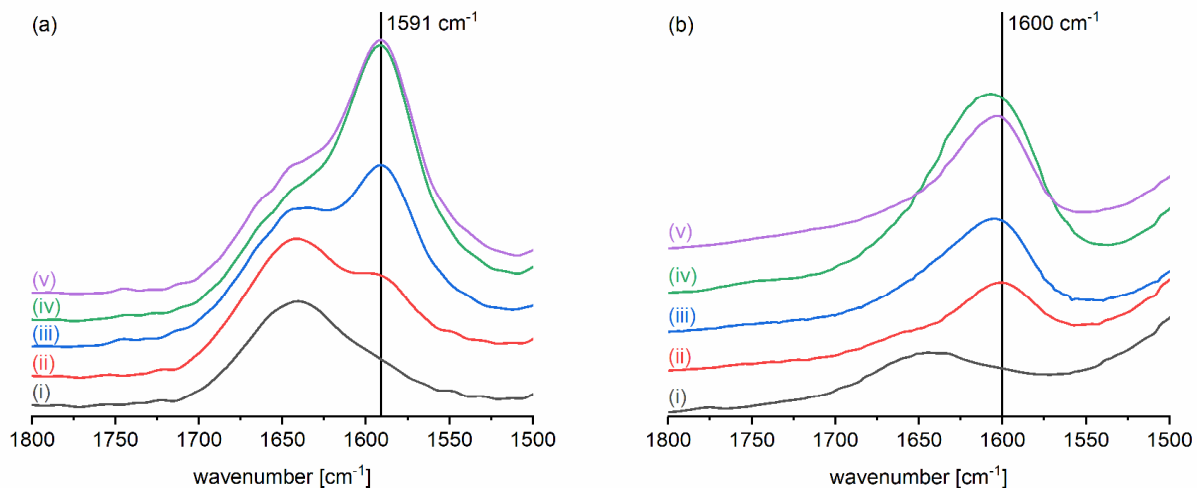


Fig. S2 The region $1500\text{--}1800 \text{ cm}^{-1}$ from FTIR spectroscopy in (a) ATR mode and (b) transmission mode (with KBr pellets). The trace labels indicate: (i) blank and demineralized samples and samples carboxymethylated in (ii) 0.5 mol/L NaOH at 30°C , (iii) in 0.5 mol/L NaOH at 50°C , (iv) in 4 mol/L NaOH at 30°C , and (v) in 4 mol/L NaOH at 50°C

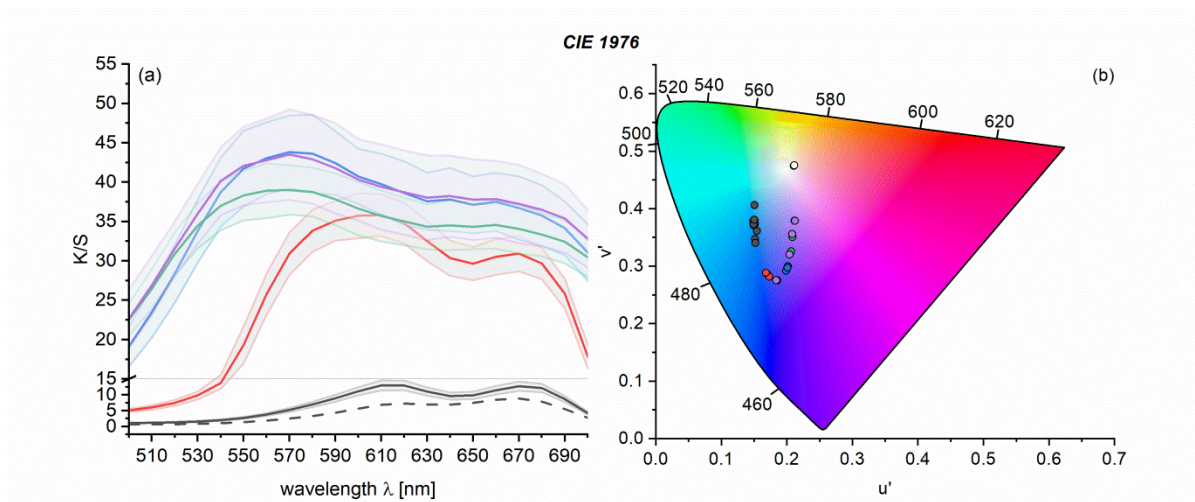


Fig. S3 (a) Absorbance spectra (as calculated with K/S_λ) from selected samples after methylene blue sorption: demineralized (---), no-MCA blank (—), carboxymethylated in 0.5 mol/L NaOH at 30°C (—), in 0.5 mol/L NaOH at 50°C (—), in 0.5 mol/L NaOH at 50°C (—), in 4 mol/L NaOH at 50°C (—) (b) color coordinates of the dyed samples plotted on CIE 1931 color space: demineralized and no-MCA blank (●), in 0.5 mol/L NaOH at 30°C (●), in 0.5 mol/L NaOH at 50°C (●), in 4 mol/L NaOH at 30°C (●) and in 4 mol/L NaOH at 50°C (●)